

A new mixing of Hartreeâ€‘Fock and local densityâ€‘fun

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#	ARTICLE	IF	CITATIONS
115	Laser flash photolysis of fluorinated aryl azides in neutral and acidic solutions. Russian Chemical Bulletin, 1990, 49, 50-55.	0.4	5
116	Isomers of C20. Dramatic effect of gradient corrections in density functional theory. Chemical Physics Letters, 1993, 214, 357-361.	1.2	144
117	Density functional thermochemistry. III. The role of exact exchange. Journal of Chemical Physics, 1993, 98, 5648-5652.	1.2	91,707
118	A general purpose exchange correlation energy functional. Journal of Chemical Physics, 1993, 99, 8765-8773.	1.2	94
119	Characterization of the potential energy surface of the HO2 molecular system by a density functional approach. Journal of Chemical Physics, 1994, 101, 10666-10676.	1.2	92
120	Inclusion of Hartree-Fock exchange in density functional methods. Hyperfine structure of second row atoms and hydrides. Journal of Chemical Physics, 1994, 101, 6834-6838.	1.2	149
121	Direct ab initio dynamics studies of proton transfer in hydrogen-bond systems. Journal of Chemical Physics, 1994, 101, 10442-10451.	1.2	126
122	Tautomeric equilibria in 2-hydroxypyridine and in cytosine. An assessment of density functional methods, including gradient corrections. Chemical Physics Letters, 1994, 220, 129-132.	1.2	49
123	Theoretical study of direct and water-assisted isomerization of formaldehyde radical cation. A comparison between density functional and post-Hartree-Fock approaches. Chemical Physics Letters, 1994, 224, 432-438.	1.2	82
124	Inclusion of Hartree-Fock exchange in the density functional approach. Benchmark computations for diatomic molecules containing H, B, C, N, O, and F atoms. Chemical Physics Letters, 1994, 226, 392-398.	1.2	84
125	Role of Hartree-Fock exchange in density functional theory. Chemical Physics Letters, 1994, 230, 189-195.	1.2	26
126	Proton transfer in model hydrogen-bonded systems by a density functional approach. Chemical Physics Letters, 1994, 231, 295-300.	1.2	99
127	The implementation of density functional theory within the polarizable continuum model for solvation. Chemical Physics Letters, 1994, 231, 34-39.	1.2	81
128	An evaluation of the performance of density functional theory, MP2, MP4, F4, G2(MP2) and G2 procedures in predicting gas-phase proton affinities. Chemical Physics Letters, 1994, 231, 345-351.	1.2	133
129	A new direct ab initio dynamics method for calculating thermal rate constants from density functional theory. Journal of Chemical Physics, 1994, 101, 7408-7414.	1.2	86
130	Theoretical calculation of vibrational circular dichroism spectra. Faraday Discussions, 1994, 99, 103.	1.6	149
131	Application of density functional methods for the study of hydrogen-bonded systems: The hydrogen fluoride dimer. Journal of Chemical Physics, 1994, 101, 9793-9799.	1.2	138
132	An implementation of analytic second derivatives of the gradient-corrected density functional energy. Journal of Chemical Physics, 1994, 100, 7429-7442.	1.2	214

#	ARTICLE	IF	CITATIONS
133	A Method for Computing One-Electron Reduction Potentials and Its Application to p-Benzoquinone in Water at 300 K. <i>Journal of the American Chemical Society</i> , 1994, 116, 11048-11051.	6.6	43
134	Pseudospectral localized Møller-Plesset methods: Theory and calculation of conformational energies. <i>Journal of Chemical Physics</i> , 1995, 103, 1481-1490.	1.2	168
135	Mechanismus der Fe ⁺ -vermittelten C-C- und C-H-Bindungsaktivierung in Ethan aus theoretischer Sicht. <i>Angewandte Chemie</i> , 1995, 107, 2430-2432.	1.6	11
136	Mechanism of the Fe ⁺ Mediated C-C and C-H Bond Activations in Ethane from a Theoretical Viewpoint. <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 2282-2285.	4.4	43
137	The water-methanol complexes. Matrix induced structural conversion of the 1-1 species. <i>Chemical Physics Letters</i> , 1995, 232, 90-98.	1.2	55
138	A density-functional study of van der Waals forces: rare gas diatomics. <i>Chemical Physics Letters</i> , 1995, 233, 134-137.	1.2	493
139	Critical assessment of density functional methods for study of proton transfer processes. (FHF) ⁺ . <i>Chemical Physics Letters</i> , 1995, 234, 159-164.	1.2	82
140	A density functional theory of the Fermi contact contribution to the nuclear spin-spin coupling constant. <i>Chemical Physics Letters</i> , 1995, 234, 319-322.	1.2	7
141	A density functional and Hartree-Fock study of pyran and 2,4-pentadienals. <i>Chemical Physics Letters</i> , 1995, 237, 45-52.	1.2	13
142	Pt ⁺ -mediated activation of methane: theory and experiment. <i>Chemical Physics Letters</i> , 1995, 239, 75-83.	1.2	110
143	The performance of density functional/Hartree-Fock hybrid methods: the bonding in cationic first-row transition metal methylene complexes. <i>Chemical Physics Letters</i> , 1995, 240, 245-252.	1.2	117
144	A new method for incorporating solvent effect into the classical, ab initio molecular orbital and density functional theory frameworks for arbitrary shape cavity. <i>Chemical Physics Letters</i> , 1995, 240, 253-260.	1.2	274
145	Gas-phase acidities: a comparison of density functional, MP2, MP4, F4, G2(MP2, SVP), G2(MP2) and G2 procedures. <i>Chemical Physics Letters</i> , 1995, 245, 123-128.	1.2	74
146	The FO ₂ radical: a new success of density functional theory. <i>Chemical Physics Letters</i> , 1995, 245, 488-497.	1.2	50
147	Investigations using the Becke-Roussel exchange functional. <i>Chemical Physics Letters</i> , 1995, 246, 381-386.	1.2	32
148	Ab initio calculation of molar volumes: Comparison with experiment and use in solvation models. <i>Journal of Computational Chemistry</i> , 1995, 16, 385-394.	1.5	90
149	Calculation of molecular geometries, relative conformational energies, dipole moments, and molecular electrostatic potential fitted charges of small organic molecules of biochemical interest by density functional theory. <i>Journal of Computational Chemistry</i> , 1995, 16, 1483-1506.	1.5	99
150	Some recent applications of ab initio electronic structure methods to metal, semimetal, and molecular clusters. <i>Structural Chemistry</i> , 1995, 6, 229-241.	1.0	2

#	ARTICLE	IF	CITATIONS
151	On the test of different atomic exchange functionals. International Journal of Quantum Chemistry, 1995, 56, 307-316.	1.0	4
152	Proton transfer in small model systems: A density functional study. International Journal of Quantum Chemistry, 1995, 56, 697-705.	1.0	27
153	Comparison of the performance of various gradient-corrected exchange and correlation functionals in density functional theory: Case studies of CO and N2O molecules. International Journal of Quantum Chemistry, 1995, 56, 753-762.	1.0	12
154	Determining and extending the domain of exchange and correlation functionals. International Journal of Quantum Chemistry, 1995, 56, 61-78.	1.0	80
155	Potential energy surfaces and vibrational spectra of H5O2+ and larger hydrated proton complexes. International Journal of Quantum Chemistry, 1995, 56, 657-668.	1.0	89
156	Charge analysis along the intrinsic reaction coordinate for the insertion reactions CFX + HY (X = H, F; Y = O, N). International Journal of Quantum Chemistry, 1995, 357, 75-86.	1.5	5
157	Structures and energetic properties of B-DNA nucleotides. Computational and Theoretical Chemistry, 1995, 357, 161-170.	1.5	16
158	Density functional study of molecular properties of hydrazoic acid and methyl azide. Computational and Theoretical Chemistry, 1995, 343, 31-41.	1.5	16
159	Validation of self-consistent hybrid density functionals for the study of structural and electronic characteristics of organic radicals. Journal of Chemical Physics, 1995, 102, 384-393.	1.2	138
160	Thermal and vibrational state selected rates of the CH4+Cl+ → HCl+CH3 reaction. Journal of Chemical Physics, 1995, 103, 9642-9652.	1.2	154
161	A hybrid density functional study of the first-row transition-metal monocarbonyls. Journal of Chemical Physics, 1995, 103, 10605-10613.	1.2	99
162	Gradient-corrected exchange potential with the correct asymptotic behavior and the corresponding exchange-energy functional obtained from the virial theorem. Physical Review A, 1995, 52, 3704-3710.	1.0	46
163	Conformational behavior of gaseous glycine by a density functional approach. Journal of Chemical Physics, 1995, 102, 364-370.	1.2	171
164	The performance of density functional/Hartree-Fock hybrid methods: Cationic transition-metal methyl complexes MCH+3 (M=Sc, Cu, La, Hf, Au). Journal of Chemical Physics, 1995, 102, 4931-4941.	1.2	150
165	Analytical first and second energy derivatives of the generalized conductorlike screening model for free energy of solvation. Journal of Chemical Physics, 1995, 103, 3709-3717.	1.2	84
166	HF Vapor. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1995, 99, 1159-1167.	0.9	42
167	π-Donor Substituent Effects on Calculated Structures and Vibrational Frequencies of p-Benzoquinone, p-Fluoranil, and p-Chloranil. The Journal of Physical Chemistry, 1995, 99, 8125-8134.	2.9	69
168	Structure, epr parameters, and reactivity of organic free radicals from a density functional approach. Theoretica Chimica Acta, 1995, 91, 113-128.	0.9	84

#	ARTICLE	IF	CITATIONS
169	Basis set convergence and performance of density functional theory including exact exchange contributions for geometries and harmonic frequencies. <i>Molecular Physics</i> , 1995, 86, 1437-1450.	0.8	164
170	Comparison of AM1 and density functional theory generated transition state structures and activation energies for cyanoalkenes addition to cyclopentadiene. <i>Computational and Theoretical Chemistry</i> , 1995, 358, 139-143.	1.5	59
171	Ab initio molecular dynamics simulation of liquid water: Comparison of three gradient-corrected density functionals. <i>Journal of Chemical Physics</i> , 1996, 105, 1142-1152.	1.2	597
172	Molecular Orbital Studies of Methoxy-1,3,5-cycloheptatriene Isomers: Results from Semiempirical, ab Initio, and Density Functional Theory Calculations. <i>Journal of Organic Chemistry</i> , 1996, 61, 969-977.	1.7	14
173	Local, Gradient-Corrected, and Hybrid Density Functional Calculations on Pd _n Clusters for n = 1-6. <i>The Journal of Physical Chemistry</i> , 1996, 100, 10827-10830.	2.9	71
174	Systematic Model Chemistries Based on Density Functional Theory: Comparison with traditional Models and with Experiment. <i>Theoretical and Computational Chemistry</i> , 1996, 4, 679-707.	0.2	39
175	How Does Fe ⁺ Activate C-C and C-H Bonds in Ethane? A Theoretical Investigation Using Density Functional Theory. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6236-6242.	2.9	163
176	The electron affinities of the silicon fluorides SiF _n (n = 1-5). <i>Journal of Chemical Physics</i> , 1996, 105, 6880-6886.	1.2	76
177	Electron Densities of Homonuclear Diatomic Molecules As Calculated from Density Functional Theory. <i>The Journal of Physical Chemistry</i> , 1996, 100, 5274-5280.	2.9	20
178	Ab Initio Study of the Mechanism of the Binding of Triplet O ₂ to Hemocyanin. <i>Inorganic Chemistry</i> , 1996, 35, 5207-5212.	1.9	47
179	Consequences of the Formation of an Organometallic Exciplex [Hg(¹ 2-arene)] in Mercury-Photosensitized Reactions of Arenes: C-C, C-O, and C-N Bond Cleavage. <i>Organometallics</i> , 1996, 15, 1157-1165.	1.1	8
180	Intermediates and Transition Structures of the Benzannulation of Heteroatom-Stabilized Chromium Carbene Complexes with Ethyne: A Density Functional Study. <i>Journal of the American Chemical Society</i> , 1996, 118, 10551-10560.	6.6	78
181	Intrinsic Aptitude of Cationic Methyl- and Ethylpalladium To Associate Ethylene and To Further Undergo Subsequent Migratory Insertion. A Theoretical Study. <i>Organometallics</i> , 1996, 15, 5542-5550.	1.1	38
182	Racemization Barriers of Helicenes: A Computational Study 1. <i>Journal of the American Chemical Society</i> , 1996, 118, 6031-6035.	6.6	203
183	Electronic Structure and Properties of Trihalogen Cations X ₃ ⁺ and XY ₂ ⁺ (X, Y = F, Cl, Br, I). <i>Inorganic Chemistry</i> , 1996, 35, 100-109.	1.9	16
184	Elementary Concepts in Density Functional Theory. <i>Theoretical and Computational Chemistry</i> , 1996, , 3-24.	0.2	12
185	Density-functional thermochemistry. IV. A new dynamical correlation functional and implications for exact-exchange mixing. <i>Journal of Chemical Physics</i> , 1996, 104, 1040-1046.	1.2	2,426
186	Observation of the Hammick Intermediate: Reduction of the Pyridine-2-ylid Ion in the Gas Phase. <i>Journal of the American Chemical Society</i> , 1996, 118, 11898-11904.	6.6	84

#	ARTICLE	IF	CITATIONS
187	Hybrid DFTâ€”MD simulations of geometry and hyperfine structure of the CCH radical in argon matrices at low temperatures. <i>Journal of Chemical Physics</i> , 1996, 105, 8195-8203.	1.2	19
188	Exploring the Boundary between Aromatic and Olefinic Character:â€” Bad News for Second-Order Perturbation Theory and Density Functional Schemes. <i>Journal of the American Chemical Society</i> , 1996, 118, 3519-3520.	6.6	57
189	Besides N ₂ , What Is the Most Stable Molecule Composed Only of Nitrogen Atoms?â€”. <i>Inorganic Chemistry</i> , 1996, 35, 7124-7133.	1.9	237
190	On hydrogen-bonded complexes: the case of (HF) ₂ . <i>Theoretica Chimica Acta</i> , 1996, 93, 61-65.	0.9	17
191	A hybrid quantum mechanical force field molecular dynamics simulation of liquid methanol: Vibrational frequency shifts as a probe of the quantum mechanical/molecular mechanical coupling. <i>Journal of Chemical Physics</i> , 1996, 104, 7261-7269.	1.2	52
192	Linear scaling computation of the Hartreeâ€”Fock exchange matrix. <i>Journal of Chemical Physics</i> , 1996, 105, 2726-2734.	1.2	212
193	Density functional study of strong hydrogenâ€”bonded systems: The hydrogen diformiate complex. <i>Journal of Chemical Physics</i> , 1996, 104, 8524-8534.	1.2	31
194	Study of NO and CO dissociation on the (100) Cu surface using density functional theory and the topological analysis of the electronic density and its Laplacian. <i>Canadian Journal of Chemistry</i> , 1996, 74, 1014-1020.	0.6	14
195	Local energy and chemical potential equations and the exchange-correlation potential. <i>Canadian Journal of Chemistry</i> , 1996, 74, 969-975.	0.6	1
196	Density functional theory study of ethene and acetylene addition to oxazole and protonated oxazole. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1996, , 1021.	0.9	39
197	Time-Dependent Density Functional Response Theory of Molecular Systems: Theory, Computational Methods, and Functionals. <i>Theoretical and Computational Chemistry</i> , 1996, , 391-439.	0.2	255
198	Pyryliumolates IIâ€”generation of and cycloaddition reactions with isoxazole annulated pyryliumolates. <i>Journal of the Chemical Society Perkin Transactions 1</i> , 1996, , 1035-1040.	0.9	20
199	â€”Iron Methoxide Cation:â€” A Simple Model To Probe the Mechanism of Î²-Hydrogen Transfer in Organometallic Compounds. <i>Journal of the American Chemical Society</i> , 1996, 118, 5047-5055.	6.6	72
200	Density functional study of isomerization of fluoro- and chloroformaldehyde radical cations. <i>Journal of Computational Chemistry</i> , 1996, 17, 1309-1317.	1.5	10
201	Inhomogeneous Electron Gas: Transcending Semiclassical Thomas-Fermi-Dirac Method. <i>Theoretical and Computational Chemistry</i> , 1996, , 67-97.	0.2	0
202	Recent Developments in Configuration Interaction and Density Functional Theory Calculations of Radical Hyperfine Structure.. <i>Advances in Quantum Chemistry</i> , 1996, 27, 297-369.	0.4	83
203	Electron Affinities of Substituted p-Benzoquinones from Hybrid Hartreeâ€”Fock/Density-Functional Calculations. <i>The Journal of Physical Chemistry</i> , 1996, 100, 10083-10087.	2.9	77
204	Rationale for mixing exact exchange with density functional approximations. <i>Journal of Chemical Physics</i> , 1996, 105, 9982-9985.	1.2	4,987

#	ARTICLE	IF	CITATIONS
205	The monochlorine fluorides (ClF _n) and their anions (ClF _n ⁻) n = 1-7: structures and energetics. <i>Molecular Physics</i> , 1996, 89, 607-631.	0.8	63
206	Density functionals: Where do they come from, why do they work?. <i>Topics in Current Chemistry</i> , 1996, , 1-30.	4.0	40
207	An assessment of density functional theory on evaluating activation barriers for small organic gas-phase rearrangement reactions. <i>Computational and Theoretical Chemistry</i> , 1996, 362, 163-173.	1.5	27
208	Performance of pure and hybrid DFT methods in calculations of ethylene iodonium and methyl iodide. <i>Computational and Theoretical Chemistry</i> , 1996, 365, 111-117.	1.5	1
209	The structure of the methanol radical cation: an artificially short C-O bond with MP2 theory. <i>Chemical Physics Letters</i> , 1996, 262, 187-193.	1.2	22
210	Density functional study of the H ₃ N ⁺ -Cl ₂ system—the importance of Hartree-Fock exchange in density functional methods. <i>Computational and Theoretical Chemistry</i> , 1996, 371, 11-16.	1.5	16
211	Applications of density functional theory approaching chemical accuracy to the study of typical carbon-carbon and carbon-hydrogen bonds. <i>Computational and Theoretical Chemistry</i> , 1996, 369, 29-37.	1.5	12
212	Density functional studies of internal rotation: formamide as a prototype of the peptide bond. <i>Computational and Theoretical Chemistry</i> , 1996, 375, 181-188.	1.5	2
213	Density functional theory and ab initio study of bond dissociation energy for peroxonitrous acid and peroxyacetyl nitrate. <i>Computational and Theoretical Chemistry</i> , 1996, 370, 65-69.	1.5	48
214	Mechanistic Details of the Fe ⁺ -Mediated C-C and C-H Bond Activations in Propane: A Theoretical Investigation. <i>Helvetica Chimica Acta</i> , 1996, 79, 1939-1956.	1.0	49
215	Wechselwirkungen in MolekÄ¼lkristallen, 111. KristallzÄ¼chtung und Strukturbestimmung von Donator/Akzeptor-Komplexen aus 1,2,4,5-Tetrakis(alkylthio)benzolen und Brom oder Iod. <i>Liebigs Annalen</i> , 1996, 1996, 2185-2194.	0.8	5
216	Models for the description of the H ₃ O ⁺ and OH ⁻ ions in water. <i>Journal of Computational Chemistry</i> , 1996, 17, 1099-1107.	1.5	11
217	An ab initio study of the dioxygen binding site of hemocyanin: A comparison between CASSCF, CASPT2, and DFT approaches. <i>International Journal of Quantum Chemistry</i> , 1996, 58, 109-119.	1.0	30
218	Comparative study of DFT methods applied to small titanium/oxygen compounds. <i>International Journal of Quantum Chemistry</i> , 1996, 59, 427-443.	1.0	53
219	Stability and structure of rare-gas ionic clusters using density functional methods: A study of helium clusters. , 1996, 60, 593-608.		23
220	On the optimal mixing of the exchange energy and the electron-electron interaction part of the exchange-correlation energy. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1375-1384.	1.0	22
221	Condensed-phase effects on the conformational equilibrium of ethylene glycol. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1651-1660.	1.0	6
222	Comparison of conventional and hybrid density functional approaches. Cationic hydrides of first-row transition metals as a case study. <i>Chemical Physics Letters</i> , 1996, 249, 290-296.	1.2	44

#	ARTICLE	IF	CITATIONS
223	Application of density functional theory /Hartree-Fock hybrid methods. Geometries and bond dissociation energies of Al ⁺ complexes. Chemical Physics Letters, 1996, 250, 387-392.	1.2	44
224	Ab initio calculation of atomic axial tensors and vibrational rotational strengths using density functional theory. Chemical Physics Letters, 1996, 252, 211-220.	1.2	427
225	On the nature of the cobalt-nitrogen bond in the CON ₂ complex. A theoretical study. Chemical Physics Letters, 1996, 254, 314-320.	1.2	0
226	Density-functional and density-functional reaction field calculations of the molecular properties of phenol. Chemical Physics Letters, 1996, 258, 436-444.	1.2	19
227	The calculation of ¹ H, ¹³ C, ¹⁴ N isotropic and anisotropic hyperfine interactions for the 3-methyl indole cation and neutral radicals using hybrid density functional methods: models for in vivo tryptophan-based radicals. Chemical Physics Letters, 1996, 260, 492-498.	1.2	22
228	The structures and relative energies of formamide (H ₂ NCHO) and radical ions H ₂ NCHO ^{•+} , H ₂ NCOH ^{•+} and H ₃ NCO ^{•+} . Chemical Physics, 1996, 202, 243-252.	0.9	3
229	Structure and anisotropy of ionic argon clusters using density functional models. Chemical Physics, 1996, 208, 25-34.	0.9	13
230	Ab initio MP2 and DFT calculations of geometry and solution tautomerism of purine and some purine derivatives. Chemical Physics, 1996, 211, 147-161.	0.9	89
231	Density functional studies of internal rotation: formamide as a prototype of the peptide bond. Journal of Molecular Structure, 1996, 375, 181-188.	1.8	9
232	Construction of the adiabatic connection. Chemical Physics Letters, 1996, 263, 499-506.	1.2	164
233	Molecular and electronic structure of 1,2-disilacyclobutabenzene. Ab initio molecular orbital and density functional study. Journal of Organometallic Chemistry, 1996, 524, 107-114.	0.8	11
234	Structure, Stability, and Bonding of Transition-Metal ^π Boryl Complexes. A Molecular Orbital Study. The Journal of Physical Chemistry, 1996, 100, 6509-6517.	2.9	68
235	Ligand Substitution: An Assessment of the Reliability of ab Initio Calculations. The Journal of Physical Chemistry, 1996, 100, 18363-18370.	2.9	22
236	Infrared Matrix Isolation Study of Acetone and Methanol in Solid Argon. The Journal of Physical Chemistry, 1996, 100, 17124-17132.	2.9	72
237	Comparisons of results from parametrized configuration interaction (PCI ⁸⁰) and from hybrid density functional theory with experiments for first row transition metal compounds. Journal of Chemical Physics, 1996, 104, 9546-9554.	1.2	103
238	Molecular Quadrupole Moments for the Series of Fluoro- and Chlorobenzenes. The Journal of Physical Chemistry, 1996, 100, 6524-6530.	2.9	82
239	Comparison of density functional and coupled cluster methods in the study of metal ^π ligand systems: Sc ^π CO ₂ and Cu ^π NO ₂ . Journal of Chemical Physics, 1996, 105, 9966-9971.	1.2	46
240	Embedded density functional approach for calculations of adsorption on ionic crystals. Journal of Chemical Physics, 1996, 104, 2946-2955.	1.2	84

#	ARTICLE	IF	CITATIONS
241	On the adiabatic connection method, and scaling of electron-electron interactions in the Thomas-Fermi limit. <i>Journal of Chemical Physics</i> , 1996, 104, 1989-1992.	1.2	55
242	Adsorption of water and methanol on zeolite Bronsted acid sites: An ab initio, embedded cluster study including electron correlation. <i>Journal of Chemical Physics</i> , 1996, 105, 3770-3776.	1.2	77
243	An ab initio study of solvent shifts in vibrational spectra. <i>Journal of Chemical Physics</i> , 1996, 105, 2961-2971.	1.2	44
244	Proton transfer in the ground and lowest excited states of malonaldehyde: A comparative density functional and post-Hartree-Fock study. <i>Journal of Chemical Physics</i> , 1996, 105, 11007-11019.	1.2	215
245	Mode-specific hydrogen tunneling in tropolone: An instanton approach. <i>Journal of Chemical Physics</i> , 1996, 104, 1203-1212.	1.2	95
246	Improving energies by using exact electron densities. <i>Physical Review A</i> , 1996, 53, R2915-R2917.	1.0	22
247	Electron Affinity of Hydrogen Peroxide and the [H ₂ O ₂]-Potential Energy Surface. A Comparative DFT and ab Initio Study. <i>The Journal of Physical Chemistry</i> , 1996, 100, 100-110.	2.9	59
248	Validation of Hybrid Density Functional/Hartree-Fock Approaches for the Study of Homogeneous Catalysis. <i>The Journal of Physical Chemistry</i> , 1996, 100, 2094-2099.	2.9	32
249	Negative Ion Thermochemistry: The Sulfur Fluorides SF _n /SF _n ⁻ (n = 1-7). <i>The Journal of Physical Chemistry</i> , 1996, 100, 6061-6068.	2.9	102
250	Electron Diffraction and Vibrational Spectra of Difluorodioxirane, CF ₂ O ₂ . <i>The Journal of Physical Chemistry</i> , 1996, 100, 3983-3988.	2.9	18
251	Density Functional Studies of Vibrational Properties of HCN, H ₂ O, CH ₂ O, CH ₄ , and C ₂ H ₄ . <i>The Journal of Physical Chemistry</i> , 1996, 100, 16530-16537.	2.9	21
252	Difficulties of Density Functional Theory in Investigating Addition Reactions of the Hydrogen Atom. <i>The Journal of Physical Chemistry</i> , 1996, 100, 18422-18425.	2.9	57
253	SCRF/Monte Carlo Study of Solvent Effects on a Polar [2+2] Cycloaddition. <i>The Journal of Physical Chemistry</i> , 1996, 100, 17490-17500.	2.9	20
254	Density functional theory, the exchange hole, and the molecular bond. <i>Theoretical and Computational Chemistry</i> , 1996, , 207-238.	0.2	11
255	Charge-Transfer Complexes: Stringent Tests for Widely Used Density Functionals. <i>The Journal of Physical Chemistry</i> , 1996, 100, 12265-12276.	2.9	188
256	The effects of electron correlation on the degree of bond alternation and electronic structure of oligomers of polyacetylene. <i>Journal of Chemical Physics</i> , 1997, 107, 6712-6721.	1.2	143
257	The current in magnetic field density functional theory and its application to the chemical shielding and magnetic susceptibility. <i>Journal of Chemical Physics</i> , 1997, 107, 7350-7359.	1.2	21
258	Application of the generalized-gradient approximation to rare-gas dimers. <i>Physical Review A</i> , 1997, 56, R2495-R2498.	1.0	110

#	ARTICLE	IF	CITATIONS
259	The ground state (1A1) and the lowest triplet state (3B1) of the phenyl cation C6H5+ revisited. Journal of Chemical Physics, 1997, 106, 7541-7549.	1.2	50
260	The electron affinities of the perfluorocarbons C2Fn, n=1-6. Journal of Chemical Physics, 1997, 107, 8536-8544.	1.2	38
261	A density functional especially designed for hydrogen-only systems. Journal of Chemical Physics, 1997, 107, 10643-10651.	1.2	50
262	Density Functional Theory: A Useful Tool for the Study of Free Radicals. Advances in Quantum Chemistry, 1997, , 293-309.	0.4	17
263	The calculation of 17O chemical shielding in transition metal oxo complexes. I. Comparison of DFT and ab initio approaches, and mechanisms of relativity-induced shielding. Journal of Chemical Physics, 1997, 106, 9201-9212.	1.2	81
264	Predicting electron affinities with density functional theory: Some positive results for negative ions. Journal of Chemical Physics, 1997, 107, 2529-2541.	1.2	114
265	Density functional theory investigation of hyperfine coupling constants in peroxy radicals. Journal of Chemical Physics, 1997, 106, 7738-7748.	1.2	40
266	Hybrid schemes combining the Hartree-Fock method and density-functional theory: Underlying formalism and properties of correlation functionals. Journal of Chemical Physics, 1997, 106, 2675-2680.	1.2	97
267	The gas-phase acidity of H3PO4. Journal of Chemical Physics, 1997, 106, 3545-3547.	1.2	34
268	Computed and measured thermal diffusion factor for CO-He mixtures: a test of recent interaction potentials. Molecular Physics, 1997, 92, 957-972.	0.8	19
269	Consistencies between experiments and quantum calculations of strained C-C single bond lengths. Chemical Communications, 1997, , 2199-2200.	2.2	24
270	Cation-Interaction in Al(L)+ Complexes (L = C6H6, C5H5N, C5H6, C4H4NH, C4H4O). Journal of Physical Chemistry A, 1997, 101, 3800-3807.	1.1	47
271	Intrinsic and Environmental Effects in the Structure and Magnetic Properties of Organic Molecular Magnets: Bis(imino)nitroxide. Journal of the American Chemical Society, 1997, 119, 10831-10837.	6.6	81
272	Computer simulation of zeolite structure and reactivity using embedded cluster methods. Faraday Discussions, 1997, 106, 79-92.	1.6	190
273	Theory of Substituent Effects on Pericyclic Reaction Rates: Alkoxy Substituents in the Claisen Rearrangement. Journal of the American Chemical Society, 1997, 119, 2877-2884.	6.6	65
274	Nature of the Transition Structure for Alkene Epoxidation by Peroxyformic Acid, Dioxirane, and Dimethyldioxirane: A Comparison of B3LYP Density Functional Theory with Higher Computational Levels. Journal of Physical Chemistry A, 1997, 101, 6092-6100.	1.1	102
275	Molecular decompositions of acetaldehyde and formamide: theoretical studies using Hartree-Fock, Moller-Plesset and density functional theories. Molecular Physics, 1997, 92, 497-502.	0.8	10
276	Experimental and theoretical study of monosubstituted guanidines by vibrational spectroscopy Part 1. Structure of cyanoguanidine. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 1357-1360.	1.7	17

#	ARTICLE	IF	CITATIONS
277	Application of the methylenology principle to substitution reactions. A theoretical study. Journal of the Chemical Society Perkin Transactions II, 1997, , 2691-2698.	0.9	10
278	Conformations and rotational barriers of 2,2-bi-1H-imidazole Semiempirical, ab initio, and density functional theory calculations. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2967-2971.	1.7	1
279	Evaluation of the performance of non-local and hybrid density functional theory methods for pi-radical hyperfine structures. Molecular Physics, 1997, 91, 827-834.	0.8	12
280	The C-H activation reaction of methane for all transition metal atoms from the three transition rows. Journal of Chemical Physics, 1997, 107, 4318-4328.	1.2	96
281	Quantum Chemical Investigation of Structures, Rotational Barriers, and Vibrational Spectra of the Rotamers of Ethyl Nitrite (CH ₃ CH ₂ ONO). Journal of Physical Chemistry A, 1997, 101, 5580-5586.	1.1	14
282	CoCF ₃ Is Really (FCo+ $\hat{A}\hat{A}$ F ₂ C). Organometallics, 1997, 16, 4020-4022.	1.1	13
283	A Comparison of the Properties of Various Fused-Ring Quinones and Their Radical Anions Using Hartree-Fock and Hybrid Hartree-Fock/Density Functional Methods. Journal of Physical Chemistry A, 1997, 101, 7154-7166.	1.1	54
284	The Structure of the Free MnF ₃ Molecule A Beautiful Example of the Jahn-Teller Effect. Journal of the American Chemical Society, 1997, 119, 9042-9048.	6.6	52
285	Geometric Structure and Torsional Potential of Biisothianaphthene. A Comparative DFT and ab Initio Study. Journal of the American Chemical Society, 1997, 119, 1360-1369.	6.6	99
286	Ab Initio Prediction of Vibrational Absorption and Circular Dichroism Spectra of Chiral Natural Products Using Density Functional Theory: \hat{A} $\hat{I}\pm$ -Pinene. Journal of Physical Chemistry A, 1997, 101, 9912-9924.	1.1	124
287	Hydrogen-bonding in glycine and malonaldehyde: Performance of the Lap1 correlation functional. Journal of Chemical Physics, 1997, 107, 6770-6781.	1.2	95
288	Distinctive Normal Harmonic Vibrations of [2.2]Paracyclophane. Journal of Physical Chemistry A, 1997, 101, 8233-8241.	1.1	32
289	Atomic Sulfur and Chlorine Interaction with Pd _n Clusters (n= 1-6): A Density Functional Study. Journal of Physical Chemistry A, 1997, 101, 1969-1974.	1.1	23
290	Ab Initio Prediction of Vibrational Absorption and Circular Dichroism Spectra of Chiral Natural Products Using Density Functional Theory: \hat{A} Camphor and Fenchone. Journal of Physical Chemistry A, 1997, 101, 6322-6333.	1.1	99
291	$\hat{I}\epsilon$ -Donor Substituent Effects on Calculated Structures, Spin Properties, and Vibrations of Radical Anions of p-Chloranil, p-Fluoranil, and p-Benzoquinone. Journal of Physical Chemistry A, 1997, 101, 8351-8359.	1.1	55
292	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 11. Migratory Insertion of Coordinated Nitric Oxide into Cobalt-Carbon Bonds. Journal of the American Chemical Society, 1997, 119, 3077-3086.	6.6	32
293	New Isomers of N ₈ without Double Bonds. Journal of Physical Chemistry A, 1997, 101, 1946-1950.	1.1	69
294	Theoretical Model for Pyruvoyl-Dependent Enzymatic Decarboxylation of $\hat{I}\pm$ -Amino Acids. Journal of the American Chemical Society, 1997, 119, 11725-11733.	6.6	41

#	ARTICLE	IF	CITATIONS
295	Density Functional Study of Hydrogen-Bonded Systems: The Water-Carbon Monoxide Complex. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5004-5009.	1.1	84
296	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 12. Intramolecular Carbon-Hydrogen Bond Activation in (Butenyl)manganese Tricarbonyl. <i>Organometallics</i> , 1997, 16, 2318-2324.	1.1	19
297	Electronic and Magnetic Properties of Neutral and Charged Quinone and Plastoquinone Radicals. <i>Journal of Physical Chemistry A</i> , 1997, 101, 9496-9504.	1.1	51
298	Mechanism of the Ta ⁺ -Mediated Activation of the C-H Bond in Methane. <i>Organometallics</i> , 1997, 16, 5244-5251.	1.1	36
299	Thermal Rates of Hydrogen Exchange of Methane with Zeolite: A Direct ab Initio Dynamics Study on the Importance of Quantum Tunneling Effects. <i>Journal of Physical Chemistry B</i> , 1997, 101, 2750-2752.	1.2	42
300	Assessment of Procedures for Calculating Radical Hyperfine Structures. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1352-1359.	1.1	75
301	Interaction of Alkene Radical Cations with Solvent Molecules As Described with Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8942-8948.	1.1	30
302	Density Functional and Hartree-Fock Calculations on the Cyclopropane Ring Intermediates Involved in the Zeolite-Catalyzed Skeletal Isomerization of Hydrocarbons and in the Carbon Isotope Scrambling in 2-Propyl Cation. <i>Journal of Physical Chemistry B</i> , 1997, 101, 5346-5351.	1.2	44
303	Importance of Quantum Effects for C-H Bond Activation Reactions. <i>Journal of the American Chemical Society</i> , 1997, 119, 9891-9896.	6.6	62
304	Gas-Phase Reactions of Fe(CH ₂ O) ⁺ and Fe(CH ₂ S) ⁺ with Small Alkanes: An Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 1997, 119, 12879-12888.	6.6	16
305	Hydrogen Migration vs Carbon Migration in Dialkylcarbenes. A Study of the Preferred Product in the Carbene Rearrangements of Ethylmethylcarbene, Cyclobutylidene, 2-Norbornylidene, and 2-Bicyclo[2.1.1]hexylidene. <i>Journal of the American Chemical Society</i> , 1997, 119, 5682-5689.	6.6	94
306	Systematic Theoretical Study of Structures and Bondings of the Charge-Transfer Complexes of Ammonia with HX, XY, and X ₂ (X and Y are Halogens). <i>Journal of Physical Chemistry A</i> , 1997, 101, 2879-2885.	1.1	41
307	Theoretical Approaches to Direct Exchange Couplings between Divalent Chromium Ions in Naked Dimers, Tetramers, and Clusters. <i>Journal of Physical Chemistry A</i> , 1997, 101, 705-712.	1.1	132
308	Effects of Sequential Ligation of Molybdenum Cation by Chalcogenides on Electronic Structure and Gas-Phase Reactivity. <i>Journal of Physical Chemistry A</i> , 1997, 101, 6252-6264.	1.1	138
309	A Quantum Chemical View of Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5383-5403.	1.1	576
310	Density functional calculations on model tyrosyl radicals. <i>Biophysical Journal</i> , 1997, 72, 1556-1567.	0.2	123
311	The ClO ₄ radical: Experiment versus theory. <i>Journal of Chemical Physics</i> , 1997, 106, 4028-4037.	1.2	26
312	A general methodology for quantum modeling of free-energy profile of reactions in solution: An application to the Menshutkin NH ₃ +CH ₃ Cl reaction in water. <i>Journal of Chemical Physics</i> , 1997, 107, 1881-1889.	1.2	79

#	ARTICLE	IF	CITATIONS
313	Comparison of Hartree-Fock, Density Functional, Møller-Plesset Perturbation, Coupled Cluster, and Configuration Interaction Methods for the Migratory Insertion of Nitric Oxide into a Cobalt-Carbon Bond. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1360-1365.	1.1	46
314	Distributions and averages of electron density parameters: Explaining the effects of gradient corrections. <i>Journal of Chemical Physics</i> , 1997, 106, 10184-10193.	1.2	144
315	Van Der Waals Interactions from Density Functional Theories. , 1997, , 337-382.		4
316	The alkali metal trifluorides $M+F_3^+$: how well can theory predict experiment?. <i>Molecular Physics</i> , 1997, 90, 515-524.	0.8	7
317	Decades of Theoretical Work on Protonated Hydrates. <i>Advances in Quantum Chemistry</i> , 1997, 28, 273-291.	0.4	27
318	Density-Functional Studies on the Structure and Vibrational Spectra of Transient Intermediates of p-Benzoquinone. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4449-4459.	1.1	72
319	Assessment of Basis Set and Functional Dependencies in Density Functional Theory: A Studies of Atomization and Reaction Energies. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1927-1934.	1.1	61
320	Antiferromagnetic Exchange Interactions from Hybrid Density Functional Theory. <i>Physical Review Letters</i> , 1997, 79, 1539-1542.	2.9	264
321	Conformational Information from Vibrational Spectra of Styrene, trans-Stilbene, and cis-Stilbene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3823-3831.	1.1	291
322	Electronic Characteristics of Arylated Tetraethynylethenes: A Cooperative Computational and Electrochemical Investigation. <i>Journal of the American Chemical Society</i> , 1997, 119, 2069-2078.	6.6	84
323	pKa Values of Amines in Water from Quantum Mechanical Calculations Using a Polarized Dielectric Continuum Representation of the Solvent. <i>Journal of Physical Chemistry B</i> , 1997, 101, 2959-2967.	1.2	132
324	A new gradient-corrected exchange-correlation density functional. <i>Molecular Physics</i> , 1997, 91, 847-860.	0.8	18
325	UPS Study of Compounds with Metal-Silicon Bonds: $M(CO)_nSiCl_3$ ($M = Co, Mn; n = 4, 5$) and $Fe(CO)_4(SiCl_3)_2$. <i>Organometallics</i> , 1997, 16, 1567-1572.	1.1	38
326	Ab initio calculation of molecule-surface binding: methyl halides on GaAs(110) surfaces. <i>Surface Science</i> , 1997, 382, 154-169.	0.8	7
327	Quantum chemical studies of the effects on silicate mineral dissolution rates by adsorption of alkali metals. <i>Geochimica Et Cosmochimica Acta</i> , 1997, 61, 2577-2587.	1.6	41
328	Calculated One-Electron Reduction Potentials and Solvation Structures for Selected p-Benzoquinones in Water. <i>Journal of Physical Chemistry B</i> , 1997, 101, 623-631.	1.2	65
329	An Ab Initio Study on the Conformational and Endo/exo Preferences of Acrylates in Diels-Alder Reactions. <i>Tetrahedron</i> , 1997, 53, 6057-6064.	1.0	23
330	Ab initio and density functional study of azidoacetone. <i>Computational and Theoretical Chemistry</i> , 1997, 397, 223-230.	1.5	5

#	ARTICLE	IF	CITATIONS
331	A Biradical Mechanism in the Diels-Alder Reactions of 5-Methylene-2(5H)-furanones: An Experimental Evidence and Theoretical Rationalization. <i>Journal of the American Chemical Society</i> , 1997, 119, 9992-10003.	6.6	41
332	Title is missing!. , 1997, 105, 351-355.		0
333	Application of quantum-chemical methods including density functional theory for the interpretation of isotropic hyperfine data. The example of azulenebenzoquinone. <i>Applied Magnetic Resonance</i> , 1997, 13, 405-413.	0.6	0
334	Restricted rotation about partial C,N double bonds. <i>Structural Chemistry</i> , 1997, 8, 217-226.	1.0	1
335	The hydrogen-bridged radical cation $[H_2O \cdots H \cdots O] \rightarrow [C \cdots OH]^+$: A combined experimental and theoretical study of its stability and dissociation chemistry. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1997, 160, 117-135.	1.9	16
336	A DFT/HF study of the potential energy surface of protonated ethane $C_2H_7^+$. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1997, 167-168, 675-687.	1.9	3
337	^{13}C NMR, ^{15}N NMR and quantum-chemical study of the tautomerism of 2-substituted 5-Me-7-OH-1,2,4-triazolo[1,5-a]pyrimidines. <i>Journal of Molecular Structure</i> , 1997, 435, 65-76.	1.8	12
338	Competitive resonance at the carbonyl group as visualized by the natural bond orbital analysis. <i>Journal of Molecular Structure</i> , 1997, 435, 123-132.	1.8	13
339	Quantum-mechanical calculations of chemical thermodynamics: Practice and limitations. <i>AICHE Journal</i> , 1997, 43, 2153-2156.	1.8	3
340	A DFT Study on the Vinylcyclopropanecarbaldehyde \rightarrow 2,5-Dihydrooxepin Hetero-Cope Type Rearrangement and on Related Reactions. <i>Liebigs Annalen</i> , 1997, 1997, 2443-2449.	0.8	26
341	The Thiazole Ylide: A Frequently Invoked Intermediate Is a Stable Species in the Gas Phase. <i>Chemistry - A European Journal</i> , 1997, 3, 232-236.	1.7	49
342	DFT- and post-HF-study on structure and electronic excitation of acyclic and cyclic sulfur diimides. <i>Journal of Physical Organic Chemistry</i> , 1997, 10, 33-41.	0.9	17
343	A critical analysis of electronic density functionals for structural, energetic, dynamic, and magnetic properties of hydrogen fluoride clusters. <i>Journal of Computational Chemistry</i> , 1997, 18, 1695-1719.	1.5	85
344	Why the generalized gradient approximation works and how to go beyond it. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 287-293.	1.0	126
345	Density functional study of Diels-Alder reactions between cyclopentadiene and substituted derivatives of ethylene. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 381-388.	1.0	39
346	Toward a general protocol for the study of static and dynamic properties of hydrogen-bonded systems. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 429-442.	1.0	24
347	First-row transition-metal hydrides: A challenging playground for new theoretical approaches. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 443-451.	1.0	65
348	Density-functional methods for the study of the ground-state vibrations of the guanidinium ion. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 725-739.	1.0	16

#	ARTICLE	IF	CITATIONS
349	Assembly and decomposition of building blocks to analyze polymer NEXAFS spectra. International Journal of Quantum Chemistry, 1997, 63, 749-765.	1.0	47
350	Force balance equations in inhomogeneous classical and quantal liquids. International Journal of Quantum Chemistry, 1997, 64, 21-29.	1.0	0
351	Computation of geometries and frequencies of singlet and triplet nitromethane with density functional theory using Gaussian-type orbitals. International Journal of Quantum Chemistry, 1997, 64, 263-269.	1.0	34
352	Coupling-constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	1.0	174
353	Density-functional method for very large systems with LCAO basis sets. , 1997, 65, 453-461.		1,426
354	The adiabatic connection method: a non-empirical hybrid. Chemical Physics Letters, 1997, 265, 115-120.	1.2	212
355	Higher-order gradient corrections for exchange-correlation functionals. Chemical Physics Letters, 1997, 266, 16-22.	1.2	31
356	On the parameterization of the local correlation functional. What is Becke-3-LYP?. Chemical Physics Letters, 1997, 268, 345-351.	1.2	865
357	Experimental and theoretical study of the dipole polarizability of ferrocene Fe(C ₅ H ₅) ₂ . Chemical Physics Letters, 1997, 272, 328-334.	1.2	28
358	Toward reliable adiabatic connection models free from adjustable parameters. Chemical Physics Letters, 1997, 274, 242-250.	1.2	706
359	Accurate theoretical structures of radical cations containing unusually long bonds: the structures of CH ₃ CH ₂ OH. ⁺ , ÅSH ₂ CH ₂ O+H ₂ . Chemical Physics Letters, 1997, 275, 28-34.	1.2	28
360	Hydrogen chemical shieldings in small molecules: a magnetic field density functional approach. Chemical Physics Letters, 1997, 279, 247-251.	1.2	11
361	KrOn ⁺ (n = 1, 2) and KrOH ⁺ are stable species in the gas phase. Chemical Physics Letters, 1997, 278, 202-208.	1.2	4
362	A corrective potential for hydrogen in density functional calculations. Chemical Physics Letters, 1997, 280, 73-78.	1.2	2
363	Density functional calculations of Van der Waals clusters: NeN ₂ ⁺ as a case study. Chemical Physics Letters, 1997, 276, 9-12.	1.2	1
364	Empirical density functionals. Chemical Physics Letters, 1998, 284, 6-11.	1.2	95
365	Density functional studies of the potential energy surface of the Ni ⁺ (CF ₃) complex. Chemical Physics Letters, 1998, 284, 339-343.	1.2	8
366	A theoretical study of the decomposition of gold(I) complexes. Chemical Physics Letters, 1998, 286, 73-78.	1.2	7

#	ARTICLE	IF	CITATIONS
367	Towards linear scaling in continuum solvent models.. Chemical Physics Letters, 1998, 293, 221-229.	1.2	34
368	Enthalpies of Sublimation and Crystal Lattice Energies of 9-Acridinamine and its Derivatives. Magyar AprÃ³vad KÃ©zlemÃ©nyek, 1998, 54, 183-187.	1.4	8
369	Title is missing!. Magyar AprÃ³vad KÃ©zlemÃ©nyek, 1998, 54, 189-195.	1.4	7
370	Calculation of Zero-Field Splittings, g-Values, and the Relativistic Nephelauxetic Effect in Transition Metal Complexes. Application to High-Spin Ferric Complexes. Inorganic Chemistry, 1998, 37, 6568-6582.	1.9	307
371	Hybrid methods: Combining density functional and wavefunction theory. , 1998, , 60-90.		5
372	Radiolysis of 2,6-di-tert-butyl-4-methylphenol (ionol) in a lipid membrane in the presence of oxygen. Mendeleev Communications, 1998, 8, 32-33.	0.6	0
373	Structures and stability of hydrated clusters of hydrogen chloride, HCl(H ₂ O) _n , n=1-5. Journal of Chemical Physics, 1998, 109, 973-977.	1.2	176
374	Role of Polar and Enthalpic Effects in the Addition of Methyl Radical to Substituted Alkenes: A Density Functional Study Including Solvent Effects. Journal of the American Chemical Society, 1998, 120, 5733-5740.	6.6	40
375	Ab initio Methods for the Study of Molecular Systems for Nanometer Technology: Toward the First-Principles Design of Molecular Computers. Annals of the New York Academy of Sciences, 1998, 852, 68-94.	1.8	15
376	Toward chemical accuracy in the computation of NMR shieldings: the PBE0 model. Chemical Physics Letters, 1998, 298, 113-119.	1.2	266
377	Molecular and electronic structure of some silacyclopropabenzene: the reversed Mills-Nixon effect. Journal of Organometallic Chemistry, 1998, 571, 65-75.	0.8	10
378	A comparative study of the electronic structure of Î±-MnS (alabandite) calculated at the Hartree-Fock and Density Functional levels of theory. Chemical Physics, 1998, 236, 97-105.	0.9	20
379	Comparison of density functional and MP2 geometry optimizations of Na(H ₂ O) _n (n = 1-3) clusters. Computational and Theoretical Chemistry, 1998, 425, 87-94.	1.5	6
380	Structural properties of protonated acyl derivatives as studied by quantum mechanics. Computational and Theoretical Chemistry, 1998, 428, 267-282.	1.5	10
381	Energies and structures of isomers of Cl ₂ O ₂ calculated by density functional methods. Computational and Theoretical Chemistry, 1998, 431, 185-189.	1.5	10
382	A computational study of imidazole, 4-nitroimidazole, 5-nitroimidazole and 4,5-dinitroimidazole. Computational and Theoretical Chemistry, 1998, 432, 41-53.	1.5	44
383	Glycine conformations: gradient-corrected DFT-studies. Computational and Theoretical Chemistry, 1998, 433, 193-201.	1.5	6
384	High accuracy studies on the ground state and transition state of SiC ₂ . Computational and Theoretical Chemistry, 1998, 454, 31-40.	1.5	11

#	ARTICLE	IF	CITATIONS
385	Hybrid Hartree-Fock/density functional (HF/DF) calculations of adiabatic electron affinities (EAad's) of neutral hydroquinone radicals of 1,4-benzoquinone (1) and 1,4-benzoquinone imine (2). Computational and Theoretical Chemistry, 1998, 454, 237-258.	1.5	10
386	Hartree-Fock study of the Si(100) reconstruction. Computational and Theoretical Chemistry, 1998, 458, 171-189.	1.5	4
387	Modelling the signatures of interstellar polycyclic aromatic hydrocarbons with quantum chemistry. Computational and Theoretical Chemistry, 1998, 458, 203-215.	1.5	18
388	Synthesis of Tetrahydro- and Dihydropyridines by Hetero Diels-Alder Reactions of Enantiopure β,β' -Unsaturated Sulfinimines. European Journal of Organic Chemistry, 1998, 1998, 1629-1637.	1.2	31
389	Implementation and validation of the Lacks-Gordon exchange functional in conventional density functional and adiabatic connection methods. Journal of Computational Chemistry, 1998, 19, 418-429.	1.5	91
390	Parallel pseudospectral electronic structure: II. Localized Møller-Plesset calculations. Journal of Computational Chemistry, 1998, 19, 1030-1038.	1.5	17
391	TheRate: Program for ab initio direct dynamics calculations of thermal and vibrational-state-selected rate constants. Journal of Computational Chemistry, 1998, 19, 1039-1052.	1.5	263
392	Theoretical determination of exact-exchange-mixing parameter employing the ionization energy theorem. International Journal of Quantum Chemistry, 1998, 69, 255-264.	1.0	6
393	Analysis of density functionals and their density tails in H ₂ . International Journal of Quantum Chemistry, 1998, 69, 541-550.	1.0	6
394	Virtual space level shifting and correlation energies. International Journal of Quantum Chemistry, 1998, 69, 581-590.	1.0	143
395	A theoretical study of rare-gas diatomic molecules with the generalized-gradient approximation to density functional theory. International Journal of Quantum Chemistry, 1998, 69, 619-627.	1.0	37
396	Density functional investigations of carboxyl free radicals: Formyloxyl, acetyloxyl, and benzoyloxyl radicals. International Journal of Quantum Chemistry, 1998, 70, 253-267.	1.0	34
397	Difficulties of density functional theory in predicting the torsional potential of 2,2'-bithiophene. , 1998, 70, 303-312.		34
398	Synthesis, structure, and chiroptical properties of the first 4-Oxa[7]Paracyclophane. Chirality, 1998, 10, 147-153.	1.3	14
399	Mechanism of methane monooxygenase - a structural and quantum chemical perspective. Journal of Biological Inorganic Chemistry, 1998, 3, 314-317.	1.1	61
400	Stability Order of Basic Peptide Conformations Reflected by Density Functional Theory. Journal of Molecular Modeling, 1998, 4, 53-60.	0.8	24
401	DFT computational study of the epoxidation of olefins with dioxiranes. Tetrahedron, 1998, 54, 6123-6134.	1.0	23
402	Hydrogen bonding effects in the epoxidation of propenol with dioxiranes. A DFT computational study. Tetrahedron, 1998, 54, 12323-12336.	1.0	31

#	ARTICLE	IF	CITATIONS
403	Polycyclic arene episulfides. Attempted synthesis, molecular orbital calculations and comparison with arene oxides. <i>Tetrahedron</i> , 1998, 54, 14283-14300.	1.0	16
404	Luminescent spectra of PbI ₂ single crystals doped by 3d-metal impurities. <i>Journal of Luminescence</i> , 1998, 79, 257-267.	1.5	25
405	Generation of neutral and cationic hydrogen shift isomers of pyridine: a combined experimental and computational investigation. <i>International Journal of Mass Spectrometry</i> , 1998, 179-180, 7-14.	0.7	54
406	Post-Hartree-Fock MP2 and density functional theory derived structure and vibrations of 1,2-dithiole-2-thione and 1,2-dithiole-3-one. <i>Vibrational Spectroscopy</i> , 1998, 16, 77-83.	1.2	11
407	Reactions of FeCF ₂ ⁺ and CoCF ₂ ⁺ with simple alkanes and olefins in the gas phase: An FTICR and density functional study. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1998, 175, 1-14.	1.9	15
408	Ab initio calculations on the diacetylene dimer: HCCCC(H)C(H)CCCH. <i>International Journal of Quantum Chemistry</i> , 1998, 66, 189-202.	1.0	11
409	Quantum mechanical calculations on biological systems. <i>Current Opinion in Structural Biology</i> , 1998, 8, 257-262.	2.6	109
410	Cycloaddition reactions of unsaturated hydrocarbons on the Si(100)-(2 \times 1) surface: theoretical predictions. <i>Surface Science</i> , 1998, 417, 169-188.	0.8	170
411	Size-Dependent Hydrogen Bonds of Cluster Ions between Phenol Cation Radicals and Water Molecules: A Molecular Orbital Study. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3798-3812.	1.1	38
412	In Situ UPS Study of the Formation of FeSi Films from Fe(SiCl ₃) ₂ (CO) ₄ . <i>Organometallics</i> , 1998, 17, 5825-5829.	1.1	13
413	Closed-form expression relating the second-order component of the density functional theory correlation energy to its functional derivative. <i>Journal of Chemical Physics</i> , 1998, 109, 6280-6286.	1.2	8
414	Synthesis, X-ray crystal structure and spectroscopic characterization of the new dithiolene [Pd(Et ₂ timdt) ₂] and of its adduct with molecular diiodine [Pd(Et ₂ timdt) ₂] \cdot I ₂ \cdot CHCl ₃ (Et ₂ timdt = monoanion of 1,3-diethylimidazolidine-2,4,5-trithione). <i>Journal of the Chemical Society Dalton Transactions</i> , 1998, 3731-3736.	1.1	32
415	Application of density functional theory to metal-containing radicals Study of the organometallic radicals GeH, GeCH ₃ and GeC ₂ H ₅ . <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 1555-1559.	1.7	10
416	Infrared and Raman Spectroscopy of Bis(4,4-dimethyl-2,5-cyclohexadien-1-ylidene). Vibrational Assignment by Hartree-Fock and Density Functional Theory Calculations and Depolarization Method. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2679-2684.	1.1	2
417	Tetraphenyldihydrocyclobutanes: what causes the extremely long 1.72 Å... C-C single bond?. <i>Chemical Communications</i> , 1998, 769-770.	2.2	30
418	New Formulas for Organozincate Chemistry. <i>Journal of the American Chemical Society</i> , 1998, 120, 4934-4946.	6.6	170
419	Computed and measured transport coefficients for CO-He mixtures: testing a density functional approach. <i>Molecular Physics</i> , 1998, 94, 605-622.	0.8	30
420	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 14. \hat{I}^2 -Hydrogen Transfer and Alkene/Alkyne Insertion at a Cationic Iridium Center. <i>Organometallics</i> , 1998, 17, 5139-5147.	1.1	29

#	ARTICLE	IF	CITATIONS
421	Theoretical Investigation of Adenine Radicals Generated in Irradiated DNA Components. <i>Journal of Physical Chemistry B</i> , 1998, 102, 10602-10614.	1.2	69
422	Potential models for simulations of the solvated proton in water. <i>Journal of Chemical Physics</i> , 1998, 109, 5547-5564.	1.2	187
423	Molecular Orbital Studies of the Intramolecular Reaction of Protonated cis- and trans-3,4-Epoxy-pentan-1-ol. <i>Journal of Organic Chemistry</i> , 1998, 63, 3875-3883.	1.7	12
424	A Simple Coupling Scheme between Hartree-Fock and Local Spin-Density Functional Theories. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3202-3208.	1.1	15
425	Assessment of a Combined QM/MM Approach for the Study of Large Nitroxide Systems in Vacuo and in Condensed Phases. <i>Journal of the American Chemical Society</i> , 1998, 120, 7069-7078.	6.6	100
426	Density Functional Calculations of Thermochemical Equilibria. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1568-1575.	1.1	7
427	Are Heterocyclic σ -Electron Aromatic Systems $\text{HC}^{\sim}\text{Ga}(\text{H})^{\sim}\text{CH}$, $\text{M}[\text{HGa}^{\sim}\text{C}(\text{H})^{\sim}\text{GaH}]$, $[\text{HGa}^{\sim}\text{C}(\text{H})^{\sim}\text{GaH}]^-$, $\text{HSi}^{\sim}\text{Ga}(\text{H})^{\sim}\text{SiH}$, $\text{M}[\text{HGa}^{\sim}\text{Si}(\text{H})^{\sim}\text{GaH}]$ ($\text{M} = \text{Li}, \text{Na}, \text{and K}$), and $[\text{HGa}^{\sim}\text{Si}(\text{H})^{\sim}\text{GaH}]^-$ Stable?. <i>Organometallics</i> , 1998, 17, 114-122.	1.1	40
428	Theoretical Study of the Mechanism of the Addition of Diazomethane to Ethylene and Formaldehyde. Comparison of Conventional ab Initio and Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10106-10112.	1.1	27
429	Effects of Ionizing Radiation on Crystalline Cytosine Monohydrate. <i>Journal of Physical Chemistry B</i> , 1998, 102, 7484-7491.	1.2	68
430	Radical Ions of Crownphanes Derived from Tetraphenylethene. Solution Structures and Ion-Pairing Phenomena. <i>Journal of Organic Chemistry</i> , 1998, 63, 8806-8814.	1.7	15
431	Experimental and Theoretical Studies of MCF_3^+ ($\text{M} = \text{Fe}$ and Co): Reactivities, Structures, and Potential Energy Surface for C^{\sim}F Activation. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3343-3351.	1.1	28
432	Novel Density Functional Methodology for the Computation of Accurate Electronic and Thermodynamic Properties of Molecular Systems and Improved Long-Range Behavior. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10404-10413.	1.1	34
433	Cleavage of C^{\sim}C and C^{\sim}F Bonds by Xe^+ and I^+ Ions in Reactions at a Fluorinated Self-Assembled Monolayer Surface: Collision Energy Dependence and Mechanisms. <i>Journal of the American Chemical Society</i> , 1998, 120, 8189-8198.	6.6	19
434	New Interpretation of the Valence Tautomerism of 1,6-Methano[10]annulenes and Its Application to Fullerene Derivatives. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3429-3437.	1.1	22
435	Oxidation and Stabilization of Unreconstructed Hydrogen- and Fluorine-Terminated $\text{Si}(100)$ Surface: A Periodic Density Functional Study. <i>Journal of Physical Chemistry B</i> , 1998, 102, 9215-9223.	1.2	9
436	Inter- and Intramolecular C^{\sim}H Activation by a Cationic Iridium(III) Center via Oxidative-Addition Reductive-Elimination and σ -Bond Metathesis Pathways. <i>Journal of the American Chemical Society</i> , 1998, 120, 6169-6170.	6.6	90
437	Electron Affinities of the Bromine Fluorides, BrFn ($n = 1^{\sim}7$). <i>Journal of the American Chemical Society</i> , 1998, 120, 11115-11121.	6.6	41
438	Ab Initio Study of the Mechanism for the Reaction of CF_2 Radicals with OH . <i>Journal of Physical Chemistry A</i> , 1998, 102, 9869-9875.	1.1	22

#	ARTICLE	IF	CITATIONS
439	Fluxionality and Isomerism of the Bis(dihydrogen) Complex RuH ₂ (H ₂) ₂ (PCy ₃) ₂ : INS, NMR, and Theoretical Studies. <i>Inorganic Chemistry</i> , 1998, 37, 3475-3485.	1.9	44
440	Vibrational Analysis of a Strongly Correlated System, Pentamethine Streptocyanine Dye, Based on Observed Infrared and Raman Spectra and Density Functional Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8413-8421.	1.1	21
441	Electrophilic and Oxidative Activation of the Central C-C Bond in [3.3.n]Propellanes: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 1998, 63, 6494-6502.	1.7	29
442	A Comprehensive Study of Sugar Radicals in Irradiated DNA. <i>Journal of Physical Chemistry B</i> , 1998, 102, 7674-7686.	1.2	48
443	Degenerate Lithium-Hydrogen Exchange Reactions: An Alternative Mechanism for Metalation of CH ₄ in Gas Phase and Tetrahydrofuran Solution. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8369-8376.	1.1	14
444	Matrix Isolation Fourier Transform Infrared and Ab Initio Studies of the 193-nm-Induced Photodecomposition of Formamide. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6643-6650.	1.1	91
445	Methane Activation by Naked Rh ⁺ Atoms. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 1998, 102, 7303-7307.	1.1	37
446	Density Functional Studies of a Heisenberg Spin Coupled Chromium-Semiquinone Complex and Its Chromium-Catechol Analog. <i>Journal of the American Chemical Society</i> , 1998, 120, 12051-12068.	6.6	91
447	Molecular excitation energies to high-lying bound states from time-dependent density-functional response theory: Characterization and correction of the time-dependent local density approximation ionization threshold. <i>Journal of Chemical Physics</i> , 1998, 108, 4439-4449.	1.2	4,596
448	A new inhomogeneity parameter in density-functional theory. <i>Journal of Chemical Physics</i> , 1998, 109, 2092-2098.	1.2	276
449	Generalized gradient approximation to the angle- and system-averaged exchange hole. <i>Journal of Chemical Physics</i> , 1998, 109, 3313-3320.	1.2	425
450	A challenge for density functionals: Self-interaction error increases for systems with a noninteger number of electrons. <i>Journal of Chemical Physics</i> , 1998, 109, 2604-2608.	1.2	524
451	Cracking of Hydrocarbons on Zeolite Catalysts: Density Functional and Hartree-Fock Calculations on the Mechanism of the β -Scission Reaction. <i>Journal of Physical Chemistry B</i> , 1998, 102, 2232-2238.	1.2	74
452	Bond length alternation and aromaticity in large annulenes. <i>Journal of Chemical Physics</i> , 1998, 108, 6681-6688.	1.2	90
453	Transition States for Alkane Oxidations by Dioxiranes. <i>Journal of Organic Chemistry</i> , 1998, 63, 6480-6483.	1.7	59
454	Ordered Structures in Polycarbonate Studied by Infrared and Raman Spectroscopy, Wide-Angle X-ray Scattering, and Differential Scanning Calorimetry. <i>Macromolecules</i> , 1998, 31, 6611-6619.	2.2	68
455	Exchange-Correlation Energy Density from Virial Theorem. <i>Journal of Physical Chemistry A</i> , 1998, 102, 4911-4917.	1.1	86
456	Tetraphenylhexaazaanthracene: A Case for Dominance of Cyanine Ion Stabilization Overwhelming 16π Antiaromaticity. <i>Journal of the American Chemical Society</i> , 1998, 120, 2989-2990.	6.6	73

#	ARTICLE	IF	CITATIONS
457	Comparison of Experimental and Calculated Hyperfine Coupling Constants. Which Radicals Are Formed in Irradiated Guanine?. <i>Journal of Physical Chemistry B</i> , 1998, 102, 9332-9343.	1.2	82
458	A Computational Study on the Reaction Mechanism of the Boultonâ~Katritzky Rearrangement. <i>Journal of the American Chemical Society</i> , 1998, 120, 13478-13484.	6.6	48
459	Superacid-Catalyzed Electrocyclization of Diphenylmethyl Cations to Fluorenes. Kinetic and Theoretical Revisit Supporting the Involvement of Ethylene Dications. <i>Journal of the American Chemical Society</i> , 1998, 120, 4629-4637.	6.6	27
460	Ab Initio Study of the Regiochemistry of 1,3-Dipolar Cycloadditions. Reactions of Diazomethane and Formonitrile Oxide with Ethene, Propene, Acrylonitrile, and Methyl Vinyl Ether. <i>Journal of Organic Chemistry</i> , 1998, 63, 7425-7436.	1.7	51
461	Radiation Products of Thymine, 1-Methylthymine, and Uracil Investigated by Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 1998, 102, 5369-5377.	1.2	83
462	Statistical Modeling of Gas-Phase Organometallic Reactions Based on Density Functional Theory:â€‰Ni+ + C3H8. <i>Journal of Physical Chemistry A</i> , 1998, 102, 395-411.	1.1	78
463	A Systematic Failing of Current Density Functionals:â€‰Overestimation of Two-Center Three-Electron Bonding Energies. <i>Journal of Physical Chemistry A</i> , 1998, 102, 7872-7877.	1.1	234
464	Theoretical Study of the Concerted and Stepwise Mechanisms of Triazolinedione Dielsâ~Alder Reactions. <i>Journal of the American Chemical Society</i> , 1998, 120, 12303-12309.	6.6	62
465	Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. <i>Journal of Chemical Physics</i> , 1998, 108, 664-675.	1.2	3,068
466	Structure and magnetic properties of benzyl, anilino, and phenoxy radicals by density functional computations. <i>Journal of Chemical Physics</i> , 1998, 109, 10244-10254.	1.2	57
467	Solvation and conformational dynamics of dicarboxylic suberic acid. <i>Journal of Chemical Physics</i> , 1998, 109, 2403-2412.	1.2	7
468	Magnetic coupling in ionic solids studied by density functional theory. <i>Journal of Chemical Physics</i> , 1998, 108, 2519-2527.	1.2	131
469	Exchange and correlation in silicon. <i>Physical Review B</i> , 1998, 57, 8972-8982.	1.1	117
470	InitialH2O-induced oxidation of C(001)-(2x1): A study with hybrid density-functional theory. <i>Physical Review B</i> , 1998, 58, 6760-6763.	1.1	24
471	The exchange energy functional in a weak magnetic field. <i>Journal of Chemical Physics</i> , 1998, 109, 2609-2613.	1.2	4
472	Towards an accurate gold carbonyl binding energy in AuCO+: Basis set convergence and a comparison between density functional and conventional methods. <i>Journal of Chemical Physics</i> , 1998, 108, 3876-3885.	1.2	27
473	The calculation of accurate 17O hyperfine coupling constants in the hydroxyl radical:â€‰A difficult problem for current quantum chemical methods. <i>Journal of Chemical Physics</i> , 1998, 109, 9451-9462.	1.2	10
474	Coupling-constant dependence of the density functional correlation energy. <i>Journal of Chemical Physics</i> , 1998, 109, 5212-5220.	1.2	22

#	ARTICLE	IF	CITATIONS
475	Analytical second derivatives of the free energy in solution by polarizable continuum models. <i>Journal of Chemical Physics</i> , 1998, 109, 6246-6254.	1.2	220
476	Exchange-correlation density functional beyond the gradient approximation. <i>Physical Review A</i> , 1998, 57, 189-199.	1.0	69
477	Ground-state energies of isoelectronic atomic series from density-functional theory: Exploring the accuracy of density functionals. <i>Physical Review A</i> , 1998, 58, 1902-1909.	1.0	26
478	THE STRUCTURE OF 3,4-DIAZA-1,6,6a ⁴ -TRITHIAPENTALENES-A COMBINED EXPERIMENTAL AND THEORETICAL STUDY. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 1998, 140, 35-52.	0.8	13
479	Spin uncoupling in surface chemisorption of unsaturated hydrocarbons. <i>Journal of Chemical Physics</i> , 1998, 108, 1193-1205.	1.2	94
480	Medium ring compounds and their anions: a systematic density functional theory study. <i>Molecular Physics</i> , 1998, 94, 767-787.	0.8	8
481	Second-Order Relations Involving Correlation Energy and its Functional Derivative. <i>Advances in Quantum Chemistry</i> , 1998, 33, 11-29.	0.4	3
482	The Thiosulfine-Dithiirane-Dithioester Manifold $R^{1}R^{2}(CS_2)$. <i>Sulfur Reports</i> , 1998, 21, 1-42.	0.7	31
483	CH ₃ Br ₂ and CH ₃ (Br)NH ₂ . <i>Main Group Chemistry</i> , 1998, 2, 323-327.	0.4	2
484	Theoretical Studies of Multiple Metal-Metal Bonds between Divalent Molybdenum Ions in Dimers, Tetramers, and Clusters. <i>Bulletin of the Chemical Society of Japan</i> , 1998, 71, 99-112.	2.0	15
485	Substituent effects on the O-H bond dissociation enthalpies in phenolic compounds: agreements and controversies + erratum. <i>Pure and Applied Chemistry</i> , 1999, 71, 1249-1256.	0.9	41
486	Influence of Nd:MgO dopants on the electrooptical effect in LiNbO ₃ single crystals. <i>Ferroelectrics</i> , 1999, 234, 89-105.	0.3	2
487	Benchmark calculations of chemical reactions in density functional theory: Comparison of the accurate Kohn-Sham solution with generalized gradient approximations for the H ₂ +H and H ₂ +H ₂ reactions. <i>Journal of Chemical Physics</i> , 1999, 111, 4056-4067.	1.2	74
488	How do coinage metal ions bind to benzene?. <i>Molecular Physics</i> , 1999, 96, 583-591.	0.8	79
489	Analytical energy gradients of a self-consistent reaction-field solvation model based on CM2 atomic charges. <i>Journal of Chemical Physics</i> , 1999, 110, 5503-5513.	1.2	39
490	Ab initio study of the magnetic interactions in the spin-ladder compound SrCu ₂ O ₃ . <i>Physical Review B</i> , 1999, 60, 3457-3464.	1.1	60
491	Kinetic energy density dependent approximations to the exchange energy. <i>Journal of Chemical Physics</i> , 1999, 111, 911-915.	1.2	83
492	Comparative study of the density-functional theory concerning the reaction pathway of Si(100)-(2 \times 1) with H ₂ O molecules. <i>Physical Review B</i> , 1999, 60, 10632-10635.	1.1	19

#	ARTICLE	IF	CITATIONS
493	A stochastic study of microsolvation. I. Structures of CO in small argon clusters. <i>Journal of Chemical Physics</i> , 1999, 111, 6897-6908.	1.2	25
494	Exact high-density limit of correlation potential for two-electron density. <i>Journal of Chemical Physics</i> , 1999, 110, 10262-10268.	1.2	54
495	Influence of hydrostatic pressure and temperature on two-photon absorption of aC60-2-thioxo-1,3-dithiole cycloadduct. <i>Physical Review B</i> , 1999, 59, 9229-9238.	1.1	96
496	The accuracy of current density functionals for the calculation of electric field gradients: A comparison with ab initio methods for HCl and CuCl. <i>Journal of Chemical Physics</i> , 1999, 111, 3357-3364.	1.2	70
497	Intermolecular forces from density functional theory. III. A multiproperty analysis for the Ar(1S)-CO(1 Σ) interaction. <i>Journal of Chemical Physics</i> , 1999, 110, 7832-7845.	1.2	36
498	Copolymerization of tetraethoxysilane and dimethyl(diethoxy)silane studied by ²⁹ Si NMR and ab initio calculations of ²⁹ Si NMR chemical shifts. <i>Polymer</i> , 1999, 40, 6933-6945.	1.8	33
499	Enthalpic anomeric effect in 2-Y-1,3-dithianes (Y = SC ₆ H ₅ , CO ₂ CH ₂ CH ₃ , and COC ₆ H ₅). Experimental and theoretical evaluation. Solvent effects. <i>Tetrahedron</i> , 1999, 55, 359-372.	1.0	17
500	IR, Raman, NMR and density functional methods in the examination of tautomerism and features of N-methyl substituted 9-acridinamine derivatives. <i>Journal of Molecular Structure</i> , 1999, 476, 45-55.	1.8	4
501	Matrix effect found in the reaction of GaCl with HCl: application of the Onsager model to describe interactions between matrices and matrix isolated species. <i>Journal of Molecular Structure</i> , 1999, 477, 221-224.	1.8	2
502	Structural chemistry of polycyclic heteroaromatic compounds. Part 10: photoelectron spectra and electronic structures of 1-substituted 1H-benzotriazoles. <i>Journal of Molecular Structure</i> , 1999, 513, 47-62.	1.8	7
503	Photoinduced nonlinear optics in Sb ₂ Se ₃ -BaCl ₂ -PbCl ₂ glasses. <i>Optical Materials</i> , 1999, 12, 429-440.	1.7	5
504	Structure and stability of the CF ₃ ²⁺ dication. <i>International Journal of Mass Spectrometry</i> , 1999, 185-187, 701-706.	0.7	14
505	Pyrazine diradicals, carbenes, ylides, and distonic ions probed by theory and experiment. <i>International Journal of Mass Spectrometry</i> , 1999, 185-187, 925-933.	0.7	22
506	Heat of formation of the SiF ₂ ²⁺ dication: a theoretical prediction. <i>International Journal of Mass Spectrometry</i> , 1999, 192, 165-171.	0.7	15
507	Synthesis of enantiomerically pure (E)-1,1,3,3,6,6-hexamethyl-1-sila-4-cycloheptene and its absolute configuration. <i>Tetrahedron: Asymmetry</i> , 1999, 10, 3483-3492.	1.8	10
508	SiON films deposited on Si(111) substrates—new promising materials for nonlinear optics. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 1999, 64, 88-98.	1.7	55
509	On the origin of apparently short carbon-carbon double bonds in transition-metal vinyl complexes. <i>Polyhedron</i> , 1999, 18, 1717-1724.	1.0	7
510	Density functional study of the Xe ₂ H ₃ ⁺ cation. <i>Chemical Physics</i> , 1999, 247, 215-224.	0.9	11

#	ARTICLE	IF	CITATIONS
511	Adiabatic ionization potential and electron affinity of formaldehyde. <i>Chemical Physics Letters</i> , 1999, 300, 553-560.	1.2	11
512	Density functional study of the hydrogen bonding: H ₂ O \cdots HO. <i>Chemical Physics Letters</i> , 1999, 303, 96-100.	1.2	67
513	On the performance of density functional theory for symmetry-breaking problems. <i>Chemical Physics Letters</i> , 1999, 302, 425-430.	1.2	128
514	DFT study on structures and vibrational frequencies of (CS ₂) ₂ $\hat{=}$. <i>Chemical Physics Letters</i> , 1999, 304, 265-270.	1.2	15
515	Connections between the correlation potential and the static correlation kernel for two-electron densities in high-density limit. <i>Chemical Physics Letters</i> , 1999, 308, 449-455.	1.2	9
516	Formation of FeSi and FeSi ₂ films from cis-Fe(SiCl ₃) ₂ (CO) ₄ by MOCVD –precursor versus substrate control. <i>Inorganica Chimica Acta</i> , 1999, 291, 380-387.	1.2	11
517	Application of density functional theory to calculation of in-crystal anionic polarizability. <i>Chemical Physics Letters</i> , 1999, 299, 51-56.	1.2	25
518	Ionic dissociation of hydrogen bromide in water clusters: a computational study. <i>Chemical Physics Letters</i> , 1999, 301, 29-36.	1.2	59
519	On the mechanism for the reaction of fluoroformyl radicals radicals with NO: a theoretical study. <i>Chemical Physics Letters</i> , 1999, 303, 664-670.	1.2	5
520	Extrapolating the correlation energy. <i>Chemical Physics Letters</i> , 1999, 307, 227-234.	1.2	18
521	Existence of hydrogen bonding between the hydroxyl radical and hydrogen peroxide: OH \cdots H ₂ O ₂ . <i>Chemical Physics Letters</i> , 1999, 309, 274-278.	1.2	21
522	A new dioxin decomposition process based on a hybrid density-functional calculation. <i>Chemical Physics Letters</i> , 1999, 310, 355-360.	1.2	20
523	Performance of a new hybrid Hartree-Fock/Kohn-Sham model (B98) in predicting vibrational frequencies, polarisabilities and NMR chemical shifts. <i>Chemical Physics Letters</i> , 1999, 311, 69-76.	1.2	26
524	Tyrosyl radical in galactose oxidase not strongly perturbed by cysteine cross-link. <i>Chemical Physics Letters</i> , 1999, 313, 374-378.	1.2	27
525	On the mechanism of the BrO+HBr reaction. <i>Chemical Physics Letters</i> , 1999, 314, 341-346.	1.2	13
526	Computational studies of the geometric and electronic structures of BF ₃ ⁺ , AlF ₃ ⁺ , CF ₃ ⁺ and SiF ₃ ⁺ . <i>Chemical Physics Letters</i> , 1999, 313, 679-684.	1.2	8
527	A reaction class approach with the integrated molecular orbital+molecular orbital methodology. <i>Chemical Physics Letters</i> , 1999, 314, 529-533.	1.2	31
528	Title is missing!. <i>Structural Chemistry</i> , 1999, 10, 29-40.	1.0	8

#	ARTICLE	IF	CITATIONS
529	Title is missing!. Structural Chemistry, 1999, 10, 105-119.	1.0	14
530	Toward reliable density functional methods without adjustable parameters: The PBE0 model. Journal of Chemical Physics, 1999, 110, 6158-6170.	1.2	14,178
531	Theoretical Studies of Solvent Effect on the Basicity of Substituted Pyridines. Journal of Physical Chemistry B, 1999, 103, 7302-7307.	1.2	96
532	UV Absorption Spectrum and Self-Reaction Kinetics of the Cyclohexadienyl Radical, and Stability of a Series of Cyclohexadienyl-Type Radicals. Journal of Physical Chemistry A, 1999, 103, 5501-5509.	1.1	55
533	Basis set effects on the stability of the Cl2O3 isomers using B3P86 and B3LYP methods of density functional theory. Computational and Theoretical Chemistry, 1999, 460, 19-25.	1.5	10
534	A molecular orbital study of the mechanism of chlorination reaction of benzene catalyzed by Lewis acid. Computational and Theoretical Chemistry, 1999, 461-462, 399-416.	1.5	25
535	Theoretical studies on π -complex formation of organocopper compounds with acetylene. The origin of nucleophilicity of organocuprates. Computational and Theoretical Chemistry, 1999, 461-462, 167-175.	1.5	19
536	Towards more reliable prediction of formaldehyde multinuclear NMR parameters and harmonic vibrations in the gas phase and solution. Computational and Theoretical Chemistry, 1999, 467, 63-78.	1.5	22
537	Ab initio and density functional theory calculations of molecular structure and vibrational spectrum of ethyl azidoacetate. Computational and Theoretical Chemistry, 1999, 469, 55-61.	1.5	2
538	Low-level DFT calculations II: molecules containing fluorine and second-row atoms. Computational and Theoretical Chemistry, 1999, 492, 113-121.	1.5	6
539	Revision and extension of the HF-CC method. Computational and Theoretical Chemistry, 1999, 493, 1-20.	1.5	6
540	An accurate density functional method for the study of magnetic properties: the PBE0 model. Computational and Theoretical Chemistry, 1999, 493, 145-157.	1.5	168
541	New aspects of H2 activation by nickel-iron hydrogenase. International Journal of Quantum Chemistry, 1999, 73, 197-207.	1.0	56
542	Thermolysis mechanism of N-acetylpropanamide. International Journal of Quantum Chemistry, 1999, 74, 337-342.	1.0	1
543	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. , 1999, 75, 889-909.		598
544	Understanding reactivity with Kohn-Sham molecular orbital theory: E2-SN2 mechanistic spectrum and other concepts. Journal of Computational Chemistry, 1999, 20, 114-128.	1.5	515
545	Chemical reactivity indexes in density functional theory. Journal of Computational Chemistry, 1999, 20, 129-154.	1.5	1,196
546	Exploring the limits of gradient corrections in density functional theory. Journal of Computational Chemistry, 1999, 20, 63-69.	1.5	83

#	ARTICLE	IF	CITATIONS
547	Compatibility of correlation-consistent basis sets with a hybrid Hartree-Fock/density functional method. <i>Journal of Computational Chemistry</i> , 1999, 20, 207-216.	1.5	37
548	Joint quantum chemical and polarizable molecular mechanics investigation of formate complexes with penta- and hexahydrated Zn ²⁺ : Comparison between energetics of model bidentate, monodentate, and through-water Zn ²⁺ binding modes and evaluation of nonadditivity effects. <i>Journal of Computational Chemistry</i> , 1999, 20, 1379-1390.	1.5	47
549	Broken symmetry approach to calculation of exchange coupling constants for homobinuclear and heterobinuclear transition metal complexes. , 1999, 20, 1391-1400.		836
550	Tungsten Carbonyl Complexes of 1H-Diphosphirenes and Diphosphirenylium Salts. <i>European Journal of Inorganic Chemistry</i> , 1999, 1999, 1479-1488.	1.0	15
551	Structural and Energetical Characterization of the Methylbutadiene-Fe(CO) ₃ Isomers and Related Reactive Intermediates with Quantum Chemical Methods. <i>European Journal of Inorganic Chemistry</i> , 1999, 1999, 1869-1880.	1.0	15
552	Substituent Effects on the Vinylcyclopropane-Cyclopentene Rearrangement - A Theoretical Study by Restricted and Unrestricted Density Functional Theory. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 215-220.	1.2	8
553	[1,3]-Sigmatropic Rearrangements of Divinylcyclopropane Derivatives and Hetero Analogs in Competition with Cope-Type Rearrangements - A DFT Study. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 1107-1114.	1.2	22
554	Spectroscopic and Theoretical Investigations of Monocyclic Dioximes and Dimethoximes with Six-, Eight-, and Ten-Membered Rings. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 1601-1609.	1.2	9
555	The Carbene/Bridgehead-Olefin Rearrangement: DFT Calculations on 1-Bicyclo[2.1.1]hexylcarbene and 1-Bicyclo[3.1.1]heptylcarbene; Rearrangement of (5-Bromobicyclo[3.1.1]heptyl)bromocarbene. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 3057-3066.	1.2	6
556	Photoelectron Spectra and Electronic Structures of a Series of Vinylogous Thioindigoid Compounds. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 3191-3197.	1.2	6
557	NMR spectroscopic and ab initio MO study of sterically hindered 2,3-disubstituted quinoxalines. <i>Journal of Physical Organic Chemistry</i> , 1999, 12, 725-733.	0.9	9
558	Molecular structure of 5-methyl thiophene acryloyl ethyl thiolester: A vibrational spectroscopic and density functional theory study. , 1999, 5, 201-218.		3
559	A combined quantum mechanics and molecular dynamics study of small Jahn-Teller distorted hydrocarbons: Another difficult test for density-functional theory. <i>Journal of Chemical Physics</i> , 1999, 110, 12059-12069.	1.2	16
560	Anion and Cation Effects on Olefin Adsorption on Silver and Copper Halides: An Ab Initio Effective Core Potential Study of π -Complexation. <i>Journal of Physical Chemistry B</i> , 1999, 103, 3206-3212.	1.2	61
561	Comparison of π -Complexations of Ethylene and Carbon Monoxide with Cu ⁺ and Ag ⁺ . <i>Industrial & Engineering Chemistry Research</i> , 1999, 38, 2720-2725.	1.8	72
562	Mössbauer Spectroscopy of the Spin Coupled Fe ²⁺ -FeNO Centers of Nitrosyl Derivatives of Deoxy Hemerythrin and Density Functional Theory of the {FeNO} ₇ (S=3/2) Motif. <i>Journal of the American Chemical Society</i> , 1999, 121, 7846-7863.	6.6	54
563	A Critical Validation of Density Functional and Coupled-Cluster Approaches for the Calculation of EPR Hyperfine Coupling Constants in Transition Metal Complexes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9966-9983.	1.1	271
564	Coumarin 153 in the gas phase: optical spectra and quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3209-3218.	1.3	94

#	ARTICLE	IF	CITATIONS
565	Adsorption of O ₂ on TiO ₂ (110): A theoretical study. <i>Journal of Chemical Physics</i> , 1999, 110, 10539-10544.	1.2	26
566	Electron affinities of the oxides of aluminum, silicon, phosphorus, sulfur, and chlorine. <i>Journal of Chemical Physics</i> , 1999, 110, 6240-6245.	1.2	44
567	Correlation energies for some two- and four-electron systems along the adiabatic connection in density functional theory. <i>Journal of Chemical Physics</i> , 1999, 110, 2828-2835.	1.2	114
568	Formation of CF ₃ O [•] in the gas phase. <i>Journal of Chemical Physics</i> , 1999, 110, 8436-8442.	1.2	11
569	A reaction class approach for modeling gas phase reaction rates. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 1061-1065.	1.3	79
570	3-Ethynylcyclopropene: a highly suspicious crystal structure. <i>Chemical Communications</i> , 1999, , 439-440.	2.2	4
571	The radical anion of acenaphthalene. <i>Chemical Communications</i> , 1999, , 2189-2190.	2.2	7
572	Reliability of hybrid density theory's semiempirical approach for evaluation of bond dissociation energies. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 369-372.	0.9	25
574	Determination of absolute configuration using circular dichroism: Tröger's Base revisited using vibrational circular dichroism. <i>Chemical Communications</i> , 1999, , 361-362.	2.2	32
575	The thermodynamic stabilities of tricyclic tetraene C ₁₂ H ₁₂ hydrocarbons. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 2377-2381.	0.9	9
576	Spin isomerisation of para-substituted phenyl cations. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 1059-1062.	0.9	48
577	Calorimetric and quantum chemical studies of some photodimers of anthracenes. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 2457-2462.	1.3	21
578	Intramolecular cycloadditions with 1-aminoisobenzofurans: a simple entry into the field of polycyclic aza-compounds. <i>Journal of the Chemical Society Perkin Transactions 1</i> , 1999, , 59-70.	0.9	12
579	Competition between Peroxy Acid Oxygens as Hydrogen Bond Acceptors in B3LYP Transition Structures for Epoxidations of Allylic Alcohols with Peroxyformic Acid. <i>Journal of Organic Chemistry</i> , 1999, 64, 3853-3860.	1.7	37
580	Relationship between the Dipole Strength of Ligand Pre-Edge Transitions and Metal-Ligand Covalency. <i>Inorganic Chemistry</i> , 1999, 38, 4854-4860.	1.9	77
581	Photoinduced two-photon absorption and second-harmonic generation in As ₂ Te ₃ -CaCl ₂ -PbCl ₂ glasses. <i>Physical Review B</i> , 1999, 60, 942-949.	1.1	95
582	Ab initio molecular orbital calculations of the NMR chemical shieldings for mannose and mannobiose. <i>Computational Materials Science</i> , 1999, 14, 248-253.	1.4	3
583	Photoinduced effects in the Sb ₂ Se ₃ -BaCl ₂ -PbCl ₂ glasses. <i>Journal of Applied Physics</i> , 1999, 85, 425-431.	1.1	68

#	ARTICLE	IF	CITATIONS
584	Structures, thermochemistry, and electron affinities of the germanium fluorides, GeFn/GeFn ⁺ (n=1-5). Journal of Chemical Physics, 1999, 111, 7945-7953.	1.2	45
585	Distortion of the amide bond in amides and lactams. Photoelectron-spectrum and electronic structure of 3,5,7-trimethyl-1-azaadamantan-2-one, the most twisted amide. Journal of the Chemical Society Perkin Transactions II, 1999, , 1313-1316.	0.9	35
586	Validity of the Minimum Polarizability Principle in Molecular Vibrations and Internal Rotations: An ab Initio SCF Study. Journal of Physical Chemistry A, 1999, 103, 9307-9312.	1.1	127
587	A Systematic Application of Density Functional Theory to Some Carbon-Containing Molecules and Their Anions. Journal of Physical Chemistry A, 1999, 103, 4065-4077.	1.1	86
588	Implicit Solvation Models: Equilibria, Structure, Spectra, and Dynamics. Chemical Reviews, 1999, 99, 2161-2200.	23.0	2,123
589	Bromine Halides: The Neutral Molecules BrClFn (n = 1-5) and Their Anions Structures, Energetics, and Electron Affinities. Journal of the American Chemical Society, 1999, 121, 6904-6910.	6.6	13
590	Theoretical studies on the adsorption of SiCl4 on the Si (100) 2x1 surface. Surface Science, 1999, 431, 186-192.	0.8	5
591	A complete basis set model chemistry. VI. Use of density functional geometries and frequencies. Journal of Chemical Physics, 1999, 110, 2822-2827.	1.2	2,451
592	Ground State of the (H2O)2+ Radical Cation: DFT versus Post-Hartree-Fock Methods. Journal of Physical Chemistry A, 1999, 103, 166-170.	1.1	232
593	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 15. Catalytic Alkane Dehydrogenation by Iridium(III) Complexes. Journal of the American Chemical Society, 1999, 121, 3992-3999.	6.6	63
594	Regioselective protonation of ferrocene in superacid and formation of a C-H-Fe bond. An experimental and theoretical study of the structure and dynamics of the ferrocenonium ion. Canadian Journal of Chemistry, 1999, 77, 628-633.	0.6	32
595	A comparison of methods for the calculation of NMR chemical shifts. Journal of Chemical Physics, 1999, 111, 1815-1822.	1.2	147
596	Calculation of atomization energies by a multiconfigurational localized perturbation theory Application for closed shell cases. Journal of Chemical Physics, 1999, 110, 1921-1930.	1.2	14
597	Density Functional Study on the Regioselectivity of Nucleophilic Attack in 1,3-Disubstituted (Diphosphino)(1-3-allyl)palladium Cations. Organometallics, 1999, 18, 4934-4941.	1.1	48
598	[4 + 2] Dimerization and Cycloaddition Reactions of 1,2-Unsaturated Selenoaldehydes and Selenoketones. Journal of Organic Chemistry, 1999, 64, 1565-1575.	1.7	35
599	Contra-Binding Rotation in Al-L Complexes (L = C6H6, C4H4O, C5H6, C4H4NH): A New Degenerate Rearrangement. Organometallics, 1999, 18, 1050-1058.	1.1	13
600	Anion Effects on the Adsorption of Acetylene by Nickel Halides. Langmuir, 1999, 15, 7647-7652.	1.6	17
601	Structure and Reactivity Studies of CoHNO+ in the Gas Phase. Journal of Physical Chemistry A, 1999, 103, 10884-10892.	1.1	1

#	ARTICLE	IF	CITATIONS
602	Ab Initio Density Functional Theory Study of the Structure and Vibrational Spectra of Cyclohexanone and its Isotopomers. <i>Journal of Physical Chemistry A</i> , 1999, 103, 527-538.	1.1	34
603	The Electron Affinities of the Selenium Fluorides SeF_n ($n = 1 \sim 7$). <i>Journal of Physical Chemistry A</i> , 1999, 103, 7496-7505.	1.1	36
604	Spectroscopic and Computational Studies of Perfluorophenyl and Perfluoro-2-naphthyl Nitrenes in Shpolskii Matrixes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5003-5010.	1.1	10
605	Mapped Interpolation Scheme for Single-Point Energy Corrections in Reaction Rate Calculations and a Critical Evaluation of Dual-Level Reaction Path Dynamics Methods. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1140-1149.	1.1	254
606	Density Functional Theory Analysis of Electronic Structure Variations across the Orthoquinone/Semiquinone/Catechol Redox Series. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4101-4112.	1.1	54
607	Fast Electron Transfer Across Semiconductor-Molecule Interfaces: GaAs/Co(Cp) $_2$ /O. <i>Journal of Physical Chemistry B</i> , 1999, 103, 2122-2141.	1.2	48
608	A Quantum-Chemical Study of the C $_2$ H $_3$ F $_2$ and C $_2$ H $_3$ Cl $_2$ Isomers and Their Interconversion. CBS-QB3 Proton Affinities of Difluoroethenes and Dichloroethenes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7872-7882.	1.1	3
609	Theoretical Characterization of the Reaction Intermediates in a Model of the Nickel-Iron Hydrogenase of <i>Desulfovibrio gigas</i> . <i>Journal of the American Chemical Society</i> , 1999, 121, 4000-4007.	6.6	191
610	Stereospecificity in Reactions of Allylstannanes with Aldehydes Explored by Electronic Structure Calculations. <i>Journal of Organic Chemistry</i> , 1999, 64, 4680-4684.	1.7	13
611	Conformational Studies of an N-Acylated Hindered Amine Light Stabilizer. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7665-7671.	1.1	4
612	Experimental and Theoretical Investigations of Ring-Expansion in 1-Methylcyclopropylcarbene. <i>Journal of Organic Chemistry</i> , 1999, 64, 5886-5895.	1.7	16
613	Formation Pathways from 2,4,5-Trichlorophenol (TCP) to Polychlorinated Dibenzo-p-dioxins (PCDDs): An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7686-7691.	1.1	46
614	Myers-Saito versus C $_2$ -C $_6$ (Schmittel) Cyclizations of Parent and Monocyclic Enyne-Allenes: Challenges to Chemistry and Computation. <i>Journal of the American Chemical Society</i> , 1999, 121, 8615-8627.	6.6	105
615	Transition Metal Polyhydride Complexes. 11. Mechanistic Studies of the Cis to Trans Isomerization of the Iridium(III) Dihydride Ir(H) $_2$ (CO)L (L = C $_6$ H $_3$ (CH $_2$ P(H) $_2$) $_2$). <i>Organometallics</i> , 1999, 18, 5682-5687.	1.1	26
616	Mechanism of Hydroxyl Radical Addition to Imidazole and Subsequent Water Elimination. <i>Journal of Physical Chemistry B</i> , 1999, 103, 5598-5607.	1.2	33
617	Complexes of Pentahydrated Zn $^{2+}$ with Guanine, Adenine, and the Guanine-Cytosine and Adenine-Thymine Base Pairs. Structures and Energies Characterized by Polarizable Molecular Mechanics and ab Initio Calculations. <i>Journal of Physical Chemistry B</i> , 1999, 103, 11415-11427.	1.2	78
618	Hydrogen Atom Addition to Hydrocarbon Guests in Radiolyzed Zeolites. <i>Journal of Physical Chemistry B</i> , 1999, 103, 9219-9230.	1.2	25
619	Influence of Electronic Correlation on Structural, Dynamic, and Elastic Properties of Mg $_2$ Si. <i>Journal of Physical Chemistry B</i> , 1999, 103, 2601-2606.	1.2	25

#	ARTICLE	IF	CITATIONS
620	Why Do Many C ₂ -Symmetric Bisphosphine Ligands Fail in Asymmetric Hydroformylation? Theory in Front of Experiment. <i>Organometallics</i> , 1999, 18, 4354-4361.	1.1	41
621	Interconversion of FeC ₂ H ₃ ⁺ and HFeC ₂ H ₂ ⁺ : An FTICR and Density Functional Study. <i>Organometallics</i> , 1999, 18, 5460-5469.	1.1	4
622	A Density-Functional Theory Investigation of the Radiation Products of l-Î±-Alanine. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4303-4308.	1.1	44
623	Gas-Phase Ni ⁺ (2D _{5/2}) + n-C ₄ H ₁₀ Reaction Dynamics in Real Time: Experiment and Statistical Modeling Based on Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7254-7267.	1.1	42
624	Elementary Element Bonds. IX. Structures of Tetrakis(trifluoromethyl)diphosphane and -diarsane: A Experimental and Theoretical Investigations. <i>Inorganic Chemistry</i> , 1999, 38, 1099-1107.	1.9	24
625	Density Functional (DFT) Study of the Anti-Syn Isomerization of the Butenyl Group in Cationic and Neutral (Butenyl)(butadiene)(monoligand)nickel(II) Complexes. <i>Organometallics</i> , 1999, 18, 3045-3060.	1.1	48
626	A Density Functional Study of the Structures and Energetics of CXBrO where X = H, Cl, and Br. <i>Journal of Physical Chemistry A</i> , 1999, 103, 916-920.	1.1	6
627	Generation, Characterization, and Reactivity of the Transition Metal σ -Benzyne Analog of Pyrazine (Fe- $\eta^{2,3}$ -Didehydropyrazine) in the Gas Phase: An Experimental and Theoretical Study. <i>Organometallics</i> , 1999, 18, 1774-1785.	1.1	9
628	The Dehydration Step in the Enzyme-Coenzyme-B ₁₂ Catalyzed Diol Dehydrase Reaction of 1,2-Dihydroxyethane Utilizing a Hydrogen-Bonded Carboxylic Acid Group as an Additional Cofactor: A Computational Study. <i>Journal of Physical Chemistry B</i> , 1999, 103, 7531-7541.	1.2	18
629	Ruthenium Complexes Containing Two Ru- σ (η^2 -Si-H) Bonds: A Synthesis, Spectroscopic Properties, Structural Data, Theoretical Calculations, and Reactivity Studies. <i>Journal of the American Chemical Society</i> , 1999, 121, 6668-6682.	6.6	104
630	Chemical Hermaphroditism: The Potential of the Cr(CO) ₃ Moiety To Stabilize Transition States and Intermediates with Anionic, Cationic, or Radical Character at the Benzylic Position. <i>Journal of the American Chemical Society</i> , 1999, 121, 3596-3606.	6.6	80
631	New [M(R, R'-thio)dt] ₂ Metal-Dithiolenes and Related Compounds (M = Ni, Pd, Pt; R, R'-thio = Monoanion) <i>Journal of the American Chemical Society</i> , 1999, 121, 7098-7107.	6.6	85
632	An Unusual Cleavage of an Energetic Carbene. <i>Journal of the American Chemical Society</i> , 1999, 121, 7150-7151.	6.6	20
633	Initial Stage of the Catalyzed Growth of SiO ₂ Films on Si(001): An ab Initio Study. <i>Journal of Physical Chemistry B</i> , 1999, 103, 11074-11077.	1.2	14
634	Conformational Fingerprints in the IR and Raman Spectra of Oligoanilines: A Combined Theoretical and Experimental Study. <i>Chemistry of Materials</i> , 1999, 11, 855-857.	3.2	13
635	Two-photon absorption and photoinduced second-harmonic generation in Sb ₂ Te ₃ -CaCl ₂ -PbCl ₂ glasses. <i>Journal of the Optical Society of America B: Optical Physics</i> , 1999, 16, 1719.	0.9	21
636	A combination of Kohn-Sham density functional theory and multi-reference configuration interaction methods. <i>Journal of Chemical Physics</i> , 1999, 111, 5645-5655.	1.2	635
637	Assessment of the Perdew-Burke-Ernzerhof exchange-correlation functional. <i>Journal of Chemical Physics</i> , 1999, 110, 5029-5036.	1.2	3,841

#	ARTICLE	IF	CITATIONS
638	Application of Molecular Orbital Theory to the Elucidation of Radical Processes Induced by Radiation Damage to DNA. <i>Theoretical and Computational Chemistry</i> , 1999, 8, 245-277.	0.2	8
639	Theoretical and Experimental Studies of the Benzene Radical Cation: Effects of Selective Deuteration. <i>Advances in Quantum Chemistry</i> , 1999, 35, 339-355.	0.4	4
641	Structure and electronic properties of silicon oxynitride as gate dielectric. , 2000, 4182, 362.		0
642	Theoretical and Experimental Studies of Third-Order Nonlinear Optical Susceptibilities of New p-N,N'-Diamethylaniline Tetrathiafulvalene Derivatives. <i>Materials Research Society Symposia Proceedings</i> , 2000, 660, .	0.1	1
644	Hydrogenation of [5]- and [6]Metacyclophane: Reactivity and Thermochemistry. <i>Chemistry - A European Journal</i> , 2000, 6, 1537-1546.	1.7	8
645	Ethylene coordination, insertion, and chain transfer at a cationic aluminum center: A comparative study with Ab Initio correlated level and density functional methods. <i>Journal of Computational Chemistry</i> , 2000, 21, 398-410.	1.5	30
646	GIAO NMR calculations for carbazole and its N-methyl and N-ethyl derivatives. Comparison of theoretical and experimental ¹³ C chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2000, 38, 149-155.	1.1	31
647	Substituent effects on OH bond strength and hyperfine properties of phenol, as model for modified tyrosyl radicals in proteins. <i>International Journal of Quantum Chemistry</i> , 2000, 76, 714-723.	1.0	68
648	Theoretical characterization of a multifunctional electrooptical molecular device: Photochemical ring-opening mechanism of indolinospirobenzopyran. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 454-467.	1.0	11
649	Theoretical predictions of the structure, gas-phase acidity, and aromaticity of tetrathiosquaric acid. <i>International Journal of Quantum Chemistry</i> , 2000, 78, 443-449.	1.0	15
650	Parallel ab initio and molecular mechanics investigation of polycordinated Zn(II) complexes with model hard and soft ligands: Variations of binding energy and of its components with number and charges of ligands. <i>Journal of Computational Chemistry</i> , 2000, 21, 1011-1039.	1.5	74
651	A mixed quantum mechanics/molecular mechanics (QM/MM) method for large-scale modeling of chemistry in protein environments. <i>Journal of Computational Chemistry</i> , 2000, 21, 1442-1457.	1.5	380
652	Proton affinity of peroxyacetyl nitrate. A computational study of topical proton affinities. <i>Journal of Mass Spectrometry</i> , 2000, 35, 1351-1359.	0.7	9
653	Chiral Dilithiomethane Derivatives: Structure Determination and Application in Stereoselective Reactions. <i>European Journal of Inorganic Chemistry</i> , 2000, 2000, 789-799.	1.0	24
654	Bounding the extrapolated correlation energy using Padé _{1/2} approximants. <i>International Journal of Quantum Chemistry</i> , 2000, 79, 222-234.	1.0	13
655	Calculations and electron spin resonance spectra of syringic and sinapinic acid. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 1210-1215.	1.0	1
659	Violenes/Cyanine Hybrids as Electrochromics Part 2: Tetrakis(4-dimethylaminophenyl)ethene and Its Derivatives. <i>Chemistry - A European Journal</i> , 2000, 6, 2618-2632.	1.7	87
660	Vibrational Circular Dichroism and Absolute Configuration of Chiral Sulfoxides: tert-Butyl Methyl Sulfoxide. <i>Chemistry - A European Journal</i> , 2000, 6, 4479-4486.	1.7	44

#	ARTICLE	IF	CITATIONS
661	Redox Switches with Chiroptical Signal Expression Based on Binaphthyl Boron Dipyrromethene Conjugates. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 3252-3255.	7.2	140
662	A Remarkable, Stable Radical-Molecule Complex: HO ₂ ...CF ₃ C(O)OH. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 4570-4571.	7.2	18
663	Why Static Molecular Parameters Cannot Characterize the Free Radical Scavenging Activity of Phenolic Antioxidants. <i>QSAR and Combinatorial Science</i> , 2000, 19, 375-379.	1.4	23
664	Influence of Non-Stoichiometric Defects on Electrooptics in KNbO ₃ . <i>Physica Status Solidi (B): Basic Research</i> , 2000, 221, 815-829.	0.7	9
665	Molecular Dynamics Geometry Simulations of the SiN _x O _y /Si<111> Interfaces. <i>Crystal Research and Technology</i> , 2000, 35, 1305-1314.	0.6	1
666	1,2,3,4-Tetra-tert-butyl-4-trimethylsilyl-4-sila-2-cyclobuten-1-yl: A Quantum Mechanical and ESR Study. <i>European Journal of Organic Chemistry</i> , 2000, 2000, 1107-1112.	1.2	9
667	GIAO-HF/DFT calculation of ¹³ C and ¹⁵ N chemical shifts for studying tautomerism and intramolecular hydrogen bonding in 2,3-disubstituted quinoxalines. <i>Journal of Physical Organic Chemistry</i> , 2000, 13, 473-479.	0.9	8
668	Conformational properties of thiophene oligomers. <i>Journal of Heterocyclic Chemistry</i> , 2000, 37, 847-853.	1.4	26
669	Preparation, chemical and crystal structures of N-(2-acetamido-3,4,6-tri-O-acetyl-2-deoxy-β-D-glucopyranosyl)pyridinium chloride. <i>Carbohydrate Research</i> , 2000, 329, 703-707.	1.1	5
670	Investigation of the effects of substitution position on the radical anions of chlorobiphenyls. <i>Chemical Physics Letters</i> , 2000, 318, 214-221.	1.2	12
671	A quantum mechanical study of the ionic interactions in model compounds of polyelectrolyte-surfactant complexes derived from polypeptides. <i>Chemical Physics Letters</i> , 2000, 319, 318-326.	1.2	17
672	Hybrid density functionals and ab initio studies of 2-pyridone-H ₂ O and 2-pyridone-(H ₂ O) ₂ . <i>Chemical Physics Letters</i> , 2000, 324, 127-136.	1.2	40
673	Stability of protein-bound glycol radical: a density functional theory study. <i>Chemical Physics Letters</i> , 2000, 328, 270-276.	1.2	31
674	DFT/B3-LYP study of the hydrogen-bonding cooperativity: application to (2-pyridone) ₂ , 2-pyridone-H ₂ O, 2-pyridone-CH ₃ OH and 2-pyridone-CH ₃ OCH ₃ . <i>Chemical Physics Letters</i> , 2000, 331, 553-560.	1.2	37
675	Artificial symmetry breaking in radicals is avoided by the use of the Ensemble-Referenced Kohn-Sham (REKS) method. <i>Chemical Physics Letters</i> , 2000, 332, 409-419.	1.2	24
676	Ab initio and density functional predictions of the structure, gas-phase acidity and aromaticity of 1,2-dithio-3,4-diselenosquaric acid. <i>Chemical Physics Letters</i> , 2000, 317, 330-337.	1.2	7
677	Time-resolved resonance Raman and density functional study of the radical cations of chlorobiphenyls. <i>Chemical Physics Letters</i> , 2000, 316, 395-403.	1.2	17
678	Non-linear optical diagnostics of phase transitions in 1,4-cis-polybutadiene polymers. <i>European Polymer Journal</i> , 2000, 36, 2591-2596.	2.6	3

#	ARTICLE	IF	CITATIONS
679	Vibrational circular dichroism, absolute configuration and predominant conformations of volatile anesthetics: enflurane. <i>Journal of Molecular Structure</i> , 2000, 550-551, 105-115.	1.8	18
680	Solid-state NMR study of structure, size and dynamics of domains in hybrid siloxane networks. <i>Polymer</i> , 2000, 41, 5269-5282.	1.8	32
681	Reactivity and endo/exo Selectivity in Diels/Alder Reaction of o-Quinodimethanes. An Experimental and DFT Computational Study. <i>Tetrahedron</i> , 2000, 56, 2547-2559.	1.0	25
682	Mechanistic Studies in the Radical Induced DNA Strand Cleavage Formation and Reactivity of the Radical Cation Intermediate. <i>Tetrahedron</i> , 2000, 56, 4117-4128.	1.0	27
683	Photoinduced anisotropy of push/pull chromophores incorporating 5-(1,3-benzodithiol-2-ylidene)-1-(4-nitrophenyl) penta-1,3-diene embedded into photopolymer oligoetheracrylate matrices. <i>Optics Communications</i> , 2000, 176, 503-511.	1.0	9
684	Structural chemistry of polycyclic heteroaromatic compounds. Part XI. Photoelectron spectra and electronic structures of tetracyclic hetarenes of the triphenylene type. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2000, 56, 1179-1190.	2.0	9
685	Heat of formation of the CF ₂ ⁺⁺ dication: a theoretical estimate. <i>International Journal of Mass Spectrometry</i> , 2000, 201, 269-275.	0.7	9
686	High-energy [C,H ₃ ,N,O] cation radicals and molecules. <i>International Journal of Mass Spectrometry</i> , 2000, 195-196, 101-114.	0.7	9
687	Formation and structural discrimination of stable halophenylum ions in the gas phase. <i>International Journal of Mass Spectrometry</i> , 2000, 195-196, 21-31.	0.7	3
688	Stereoselective synthesis of cyclobutyl \pm -aminocyclopropyl carboxylic acid derivatives. <i>Tetrahedron: Asymmetry</i> , 2000, 11, 4903-4914.	1.8	15
689	Protonation sites in methyl nitrate and the formation of transient CH ₄ NO ₃ radicals. A neutralization/reionization mass spectrometric and computational study. <i>Journal of the American Society for Mass Spectrometry</i> , 2000, 11, 380-392.	1.2	9
690	Proton affinity of uracil. A computational study of protonation sites. <i>Journal of the American Society for Mass Spectrometry</i> , 2000, 11, 1065-1071.	1.2	74
691	An experimental and theoretical study of the valence shell photoelectron spectrum of the chlorobenzene molecule. <i>Chemical Physics</i> , 2000, 254, 385-405.	0.9	40
692	An experimental and theoretical study of the valence shell photoelectron spectrum of bromobenzene. <i>Chemical Physics</i> , 2000, 252, 257-278.	0.9	29
693	O=O bond splitting mechanism in cytochrome oxidase. <i>Journal of Inorganic Biochemistry</i> , 2000, 80, 261-269.	1.5	83
694	Frozen orbital QM/MM methods for density functional theory. <i>Chemical Physics Letters</i> , 2000, 321, 113-120.	1.2	97
695	Collisional activation of protonated halogeno-pyridines: different behaviour of target gases. <i>Chemical Physics Letters</i> , 2000, 323, 71-78.	1.2	10
696	Density functional theory and resonance Raman investigation of the ultraviolet electronic excited states of CF ₂ I ₂ . <i>Chemical Physics Letters</i> , 2000, 316, 524-530.	1.2	22

#	ARTICLE	IF	CITATIONS
697	Insights from Coulomb and exchange intracules. Computational and Theoretical Chemistry, 2000, 506, 303-312.	1.5	26
698	Approximate but realistic estimates of bond properties in alkylamines. Computational and Theoretical Chemistry, 2000, 531, 387-399.	1.5	3
699	An ab initio molecular orbital theory and density functional theory study of the conformational free energies of methyltetrahydro-2H-thiopyrans. Computational and Theoretical Chemistry, 2000, 529, 225-239.	1.5	17
700	Solvent effects on the relative stability of 4-nitro-1 H -imidazole and 5-nitro-1 H -imidazole. Ab initio and density functional theory calculations. Computational and Theoretical Chemistry, 2000, 532, 279-286.	1.5	11
701	The gas-phase acidity and aromaticity of squaric acid: an ab initio and density functional theory study. Computational and Theoretical Chemistry, 2000, 497, 137-144.	1.5	36
702	Theoretical study of the hydrogen bonded structures between H ₂ S and OH radical. Computational and Theoretical Chemistry, 2000, 505, 241-246.	1.5	11
703	The role of the kinetic energy density in approximations to the exchange energy. Computational and Theoretical Chemistry, 2000, 501-502, 59-64.	1.5	28
704	Shell structure in free and confined atoms using the density functional theory. Computational and Theoretical Chemistry, 2000, 501-502, 183-188.	1.5	24
705	Title is missing!. Structural Chemistry, 2000, 11, 155-160.	1.0	30
706	Title is missing!. Magyar Apr ³ vd K ^z lem [©] nyek, 2000, 60, 927-941.	1.4	12
707	Theoretical and Experimental Investigations of The Decomposition of 10-methylacridinium Halides. Magyar Apr ³ vd K ^z lem [©] nyek, 2000, 60, 35-43.	1.4	3
708	The Chemical State of Sulfur in Cadmium Dithiocarbamate. Journal of Structural Chemistry, 2000, 41, 934-938.	0.3	0
709	A Theoretical Study of the Excited States of Chlorophylla and Pheophytina. Journal of Physical Chemistry B, 2000, 104, 5395-5398.	1.2	95
710	Unimolecular Decomposition of the 2-Oxepinoxy Radical: A Key Seven-Membered Ring Intermediate in the Thermal Oxidation of Benzene. Journal of Physical Chemistry A, 2000, 104, 8121-8130.	1.1	40
711	Simulation of thermoelectric properties of bismuth telluride single crystalline films grown on Si and SiO ₂ surfaces. Physical Review B, 2000, 62, 17108-17114.	1.1	23
712	Prediction of the Raman spectrum of the aqueous formate anion by a combined density functional theory and self-consistent-reaction-field study. Theoretical Chemistry Accounts, 2000, 105, 68-76.	0.5	27
713	Theoretical and Experimental Studies of Third-Order Nonlinear Optical Susceptibilities of New p-N,N'-Diamethylaniline Tetrathiafulvalene Derivatives. Materials Research Society Symposia Proceedings, 2000, 660, 1.	0.1	1
714	High-level Computational Study of the Site-, Facial- and Stereoselectivities for the Diels-Alder Reaction Between o-Benzoquinone and Norbornadiene. Molecules, 2000, 5, 1417-1428.	1.7	10

#	ARTICLE	IF	CITATIONS
715	From Classical Density Functionals to Adiabatic Connection Methods. The State of the Art.. Advances in Quantum Chemistry, 2000, 36, 45-75.	0.4	53
716	A theoretical study of the reaction of Ti+ with ethane. Journal of Chemical Physics, 2000, 112, 10247-10258.	1.2	28
717	A combined reaction class approach with integrated molecular orbital+molecular orbital (IMOMO) methodology: A practical tool for kinetic modeling. Journal of Chemical Physics, 2000, 112, 24-30.	1.2	24
718	Density functionals for the strong-interaction limit. Physical Review A, 2000, 62, .	1.0	96
719	New $\bar{\lambda}$ -dependent correlation functional combined with a modified Becke exchange. Journal of Chemical Physics, 2000, 113, 10013-10027.	1.2	79
720	Simulation of delocalized exchange by local density functionals. Journal of Chemical Physics, 2000, 112, 4020-4026.	1.2	165
721	The Hartree product and the description of local and global quantities in atomic systems: A study within Kohn-Sham theory. Journal of Chemical Physics, 2000, 112, 1150-1157.	1.2	22
722	Improved quantum mechanical study of the potential energy surface for the bithiophene molecule. Journal of Chemical Physics, 2000, 113, 4206-4215.	1.2	61
723	An exchange functional for accurate virtual orbital energies. Journal of Chemical Physics, 2000, 112, 7002-7007.	1.2	11
724	Efficient pseudospectral methods for density functional calculations. Journal of Chemical Physics, 2000, 112, 10131-10141.	1.2	32
725	Photoisomerization reaction of CH ₂ BrI following A-band and B-band photoexcitation in the solution phase: Transient resonance Raman observation of the iso-CH ₂ I-Br photoproduct. Journal of Chemical Physics, 2000, 113, 3194-3203.	1.2	53
726	Exchange energy in the local Airy gas approximation. Physical Review B, 2000, 62, 10046-10050.	1.1	98
727	Transient resonance Raman spectroscopy and density functional theory investigation of iso-polyhalomethanes containing bromine and/or iodine atoms. Journal of Chemical Physics, 2000, 113, 10934-10946.	1.2	47
728	The optimized effective potential and the self-interaction correction in density functional theory: Application to molecules. Journal of Chemical Physics, 2000, 112, 7880-7890.	1.2	96
729	Complete basis set extrapolations for low-lying triplet electronic states of acetylene and vinylidene. Journal of Chemical Physics, 2000, 113, 1447-1454.	1.2	24
730	An extensive study of gradient approximations to the exchange-correlation and kinetic energy functionals. Journal of Chemical Physics, 2000, 112, 5639-5653.	1.2	43
731	Linear scaling computation of the Fock matrix. V. Hierarchical Cubature for numerical integration of the exchange-correlation matrix. Journal of Chemical Physics, 2000, 113, 10037-10043.	1.2	43
732	Modeling proton mobility in acidic zeolite clusters. I. Convergence of transition state parameters from quantum chemistry. Journal of Chemical Physics, 2000, 112, 6779-6786.	1.2	33

#	ARTICLE	IF	CITATIONS
733	Exchange-correlation hole of the Si atom: a quantum Monte Carlo study. <i>Physical Review A</i> , 2000, 62, .	1.0	9
734	A stochastic study of microsolvation. II. Structures of CO in small helium clusters. <i>Journal of Chemical Physics</i> , 2000, 112, 2239-2250.	1.2	36
735	Perspective on inhomogeneous electron gas, 2000, , 259-262.		4
736	Photoinduced optical second-harmonic generation of SiNO films deposited on Si ¹¹¹ substrate. <i>Journal of Applied Physics</i> , 2000, 87, 3806-3814.	1.1	11
737	A density functional theory study of the nonlocal effects of NH ₃ adsorption and dissociation on Si(100)-(2 \times 1). <i>Surface Science</i> , 2000, 469, 9-20.	0.8	110
738	Elliptically polarized light-induced second harmonic generation in SiN _x O _y . <i>Journal of Non-Crystalline Solids</i> , 2000, 262, 143-154.	1.5	8
739	Intrinsic acidity of aluminum, chromium (III) and iron (III) $\frac{1}{4}$ -hydroxo functional groups from ab initio electronic structure calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2000, 64, 1675-1680.	1.6	28
740	Hexacarbonyldiplatinum(I). Synthesis, Spectroscopy, and Density Functional Calculation of the First Homoleptic, Dinuclear Platinum(I) Carbonyl Cation, [Pt(CO) ₃] ₂ ²⁺ , Formed in Concentrated Sulfuric Acid. <i>Journal of the American Chemical Society</i> , 2000, 122, 6862-6870.	6.6	52
741	An experimental and theoretical approach to the study of the properties of parabanic acid and related compounds: synthesis and crystal structure of diethylimidazolidine-2-selone-4,5-dione. <i>Canadian Journal of Chemistry</i> , 2000, 78, 1147-1157.	0.6	11
742	Conjugation Involving Nitrogen Lone-Pair Electrons: Can It Lead to Stable Multiply Charged Cations?. <i>Inorganic Chemistry</i> , 2000, 39, 3718-3721.	1.9	18
743	Theoretical Studies on Reactions of Transition-Metal Complexes. <i>Chemical Reviews</i> , 2000, 100, 353-406.	23.0	811
744	Regioselectivity and Diastereoselectivity in the 1,3-Dipolar Cycloadditions of Nitrones with Acrylonitrile and Maleonitrile. The Origin of ENDO/EXO Selectivity##Dedicated to professor G.Del Re. <i>Advances in Quantum Chemistry</i> , 2000, 36, 151-167.	0.4	16
745	Computational Studies of the Mechanism for Proton and Hydride Transfer in Liver Alcohol Dehydrogenase. <i>Journal of the American Chemical Society</i> , 2000, 122, 4803-4812.	6.6	168
746	Interpretation of the electronic absorption spectrum of free-base porphin using time-dependent density-functional theory. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2275-2281.	1.3	109
747	Thermodynamics of the Photoenzymic Repair Mechanism Studied by Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2000, 122, 10126-10132.	6.6	49
748	Catalytic Mechanism of Galactose Oxidase: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2000, 122, 8031-8036.	6.6	134
749	Electronic Structure of Activated Bleomycin: Oxygen Intermediates in Heme versus Non-Heme Iron. <i>Journal of the American Chemical Society</i> , 2000, 122, 11703-11724.	6.6	147
750	Rearrangement Pathways of Arylperoxy Radicals. 2. Five-Membered Heterocycles. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6324-6331.	1.1	13

#	ARTICLE	IF	CITATIONS
751	Effects of Alkyl Substituents on the Excited States of Naphthalene: A Semiempirical Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1020-1029.	1.1	10
752	The meta-GGA functional: Thermochemistry with a kinetic energy density dependent exchange-correlation functional. <i>Journal of Chemical Physics</i> , 2000, 112, 2643-2649.	1.2	114
753	What correlation effects are covered by density functional theory?. <i>Molecular Physics</i> , 2000, 98, 1639-1658.	0.8	55
754	X-Ray structures and ab initio study of the conformational properties of novel oxazole and thiazole containing di- and tripeptide mimetics. <i>Perkin Transactions II RSC</i> , 2000, , 1081-1085.	1.1	10
755	Computational Study of the Electronic Structure of Substituted Phenylcarbene in the Gas Phase. <i>Journal of Organic Chemistry</i> , 2000, 65, 8348-8356.	1.7	72
756	Electron Affinities of Silicon Hydrides: SiH_n ($n = 0 \sim 4$) and Si_2H_n ($n = 0 \sim 6$). <i>Journal of Physical Chemistry A</i> , 2000, 104, 11232-11242.	1.1	90
757	Gas-Phase Coordination of Mg^+ , $(\text{c-C}_5\text{H}_5)\text{Mg}^+$, and $(\text{c-C}_5\text{H}_5)_2\text{Mg}^+$ with Saturated Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3926-3932.	1.1	20
758	Equilibria of simple thioenol/thiocarbonyl pairs. Comparison with the oxygen analogs and with the parent selenium and tellurium systems. A theoretical study. <i>Perkin Transactions II RSC</i> , 2000, , 2269-2279.	1.1	17
759	Representation of potential energy surfaces by discrete polynomials: proton transfer in malonaldehyde. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 4095-4103.	1.3	12
760	Bacteriochlorophyll a radical cation and anion calculation of isotropic hyperfine coupling constants by density functional methods. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 4772-4778.	1.3	16
761	Ab Initio Studies of Benzocyclopropanone, Benzocyclopropanone-Containing [2.2]paracyclophane, Its Benzyne Derivative, and the Bridged Benzobarrelene Formed by Intramolecular [4 + 2]Cycloaddition. <i>Journal of Organic Chemistry</i> , 2000, 65, 6620-6626.	1.7	3
762	Dynamics of Chemical and Charge-Transfer Reactions of Molecular Dications: III. Beam Scattering and Total Cross Section Data for Processes in the System $\text{CO}_2^{2+} + \text{D}_2$. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7294-7303.	1.1	47
763	Structures, Intramolecular Rotation Barriers, and Thermodynamic Properties (Enthalpies, Entropies) of C_6H_6^+ . <i>Journal of Physical Chemistry A</i> , 2000, 104, 8270-8282.	1.1	36
764	Ab Initio Study of Adsorption and Decomposition of NH_3 on $\text{Si}(100)-(2 \times 1)$. <i>Journal of Physical Chemistry B</i> , 2000, 104, 2527-2533.	1.2	118
765	Ab Initio Calculations on Reactions of CHF_3 with Its Fragments. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2729-2733.	1.1	11
766	Theoretical Study of Ruthenium-Catalyzed Hydrogenation of Carbon Dioxide into Formic Acid. Reaction Mechanism Involving a New Type of σ -Bond Metathesis. <i>Journal of the American Chemical Society</i> , 2000, 122, 3867-3877.	6.6	132
767	Aromatics/Aliphatics Separation by Adsorption: New Sorbents for Selective Aromatics Adsorption by π -Complexation. <i>Industrial & Engineering Chemistry Research</i> , 2000, 39, 3856-3867.	1.8	72
768	Cyclic In-Plane Electron Delocalization (π -Bishomoaromaticity) in $4N/5e$ Radical Anions and $4N/6e$ Dianions: Generation, Structures, Properties, Ion-Pairing, and Calculations. <i>Journal of the American Chemical Society</i> , 2000, 122, 10650-10660.	6.6	21

#	ARTICLE	IF	CITATIONS
769	Effects of Gas-Phase Basicity on the Proton Transfer between Organic Bases and Trifluoroacetic Acid in the Gas Phase: Energetics of Charge Solvation and Salt Bridges. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10271-10279.	1.1	24
770	Oxidative Degradation of Pyruvate Formate-Lyase. <i>Journal of the American Chemical Society</i> , 2000, 122, 2035-2040.	6.6	27
771	Computational Study of the Unimolecular Decomposition Pathways of Phenylperoxy Radical. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3004-3011.	1.1	62
772	New Radical-Molecule Association Compounds. <i>Journal of the American Chemical Society</i> , 2000, 122, 9196-9200.	6.6	25
773	Vibrational Spectra and Structures of Long-Chain Streptocyanine Dyes: Effects of Electron-Vibration Interactions and Vibrational Polarizabilities. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11203-11211.	1.1	11
774	Ab Initio Calculation of Homogeneous Outer Sphere Electron Transfer Rates: Application to $M(OH_2)_6^{3+/2+}$ Redox Couples. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6718-6725.	1.1	67
775	Solvation of the Hydroxide Anion: A Combined DFT and Molecular Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2384-2395.	1.1	54
776	Transition Metal Polyhydride Complexes. 10. Intramolecular Hydrogen Exchange in the Octahedral Iridium(III) Dihydrogen Dihydride Complexes $IrXH_2(\eta^2-H_2)(PR_3)_2$ ($X = Cl, Br, I$). <i>Journal of the American Chemical Society</i> , 2000, 122, 2903-2910.	6.6	38
777	On the Z-E Photoisomerization of Chiral 2-Pentenoate Esters: Stationary Irradiations, Laser-Flash Photolysis Studies, and Theoretical Calculations. <i>Journal of Organic Chemistry</i> , 2000, 65, 6958-6965.	1.7	12
778	Rearrangement Pathways of Arylperoxy Radicals. I. The Azabenzenes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6088-6094.	1.1	11
779	Catalysis Mediated by Hydrogen Bonding: A Computational Study of the Aminolysis of 6-Chloropyrimidine. <i>Journal of the American Chemical Society</i> , 2000, 122, 5384-5386.	6.6	8
780	Density Functional Theory Study of the Hydrogen-Bonded Pyridine-H ₂ O Complex: A Comparison with RHF and MP2 Methods and with Experimental Data. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2112-2119.	1.1	125
781	Structures of Protonated Arginine Dimer and Bradykinin Investigated by Density Functional Theory: Further Support for Stable Gas-Phase Salt Bridges. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6069-6076.	1.1	70
782	Reaction Path Hamiltonian Analysis of Dynamical Solvent Effects for a Claisen Rearrangement and a Diels-Alder Reaction. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8058-8066.	1.1	37
783	Density Functional Calculation of the Electric Field Gradient in Cadmium Complexes: Comparison with Hartree-Fock, Second-Order Møller-Plesset, and Experimental Results. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6047-6055.	1.1	17
784	Theoretical Studies of the Radiation Products of Hydroxyproline. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8583-8592.	1.1	20
785	Epoxidation of Acyclic Chiral Allylic Alcohols with Peroxy Acids: Spiro or Planar Butterfly Transition Structures? A Computational DFT Answer. <i>Journal of Organic Chemistry</i> , 2000, 65, 2030-2042.	1.7	28
786	A Density Functional Theory Study of the Radiation Products of Glycine. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5080-5086.	1.1	36

#	ARTICLE	IF	CITATIONS
787	The First Density Functional Study on the [4 + 2]-Cycloaddition Reactions of 1,2-Diaza-1,3-butadiene with Alkenes. <i>Journal of Organic Chemistry</i> , 2000, 65, 8251-8259.	1.7	13
788	The Elusive Formaldonitrone, CH ₂ N(H)O. Preparation in the Gas Phase and Characterization by Variable-Time Neutralization-Reionization Mass Spectrometry, and Ab Initio and Density Functional Theory Calculations. <i>Journal of the American Chemical Society</i> , 2000, 122, 525-531.	6.6	24
789	Solvation Can Open the Photoisomerization Pathway for the Direct Photodissociation Reaction of Diiodomethane: A Transient Resonance Raman Observation of the Isodiiodomethane Photoproduct from Ultraviolet Excitation of Diiodomethane in the Solution Phase. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6880-6886.	1.1	81
790	How Strong Is the C ₁ ±H ₁ ·OC Hydrogen Bond?. <i>Journal of the American Chemical Society</i> , 2000, 122, 4750-4755.	6.6	402
791	Electronic Structure of Diatomic Molecules Composed of a First-Row Transition Metal and Main-Group Element (H ₁ F). <i>Chemical Reviews</i> , 2000, 100, 679-716.	23.0	302
792	Mechanism and Quantum Mechanical Tunneling Effects on Inner Hydrogen Atom Transfer in Free Base Porphyrin: A Direct ab Initio Dynamics Study. <i>Journal of the American Chemical Society</i> , 2000, 122, 897-906.	6.6	60
793	Comparison of the Accurate Kohn-Sham Solution with the Generalized Gradient Approximations (GGAs) for the SN ₂ Reaction F ⁻ + CH ₃ F → FCH ₃ + F: A Qualitative Rule To Predict Success or Failure of GGAs. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8558-8565.	1.1	151
794	Mechanisms of Hydrogen Exchange of Methane with H-Zeolite Y: An ab Initio Embedded Cluster Study. <i>Journal of Physical Chemistry B</i> , 2000, 104, 6308-6312.	1.2	53
795	Solvation Effects on the A-Band Photodissociation of Dibromomethane: Turning a Photodissociation into a Photoisomerization. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10464-10470.	1.1	38
796	On the Behavior of $\hat{I}_{\pm, \hat{I}}^2$ -Unsaturated Thioaldehydes and Thioketones in the Diels-Alder Reaction. <i>Journal of Organic Chemistry</i> , 2000, 65, 6601-6612.	1.7	33
797	Intramolecular Proton Transfer in Glycine Radical Cation. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1256-1261.	1.1	59
798	Importance of Charge Transfer and Polarization Effects for the Modeling of Uranyl ⁺ Cation Complexes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4095-4101.	1.1	63
799	Many-Body Effects in Systems of Peptide Hydrogen-Bonded Networks and Their Contributions to Ligand Binding: A Comparison of the Performances of DFT and Polarizable Molecular Mechanics. <i>Journal of Physical Chemistry B</i> , 2000, 104, 9746-9754.	1.2	93
800	Temperature Dependence of the HO ₂ + ClO Reaction. 1. Reaction Kinetics by Pulsed Photolysis-Ultraviolet Absorption and ab Initio Studies of the Potential Surface. <i>Journal of Physical Chemistry A</i> , 2000, 104, 308-319.	1.1	35
801	Reactions of Nitromethane on Si(100): First-Principles Predictions. <i>Journal of Physical Chemistry B</i> , 2000, 104, 12269-12274.	1.2	43
802	A DFT/MRCI study on the excited state charge transfer states of N-pyrrolobenzene, N-pyrrolobenzonitrile and 4-N,N-dimethylaminobenzonitrile. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 5545-5552.	1.3	77
803	Ab initio study of the reaction of a Si(001) $\hat{I}^{\sim}(2\hat{A}-1)$ surface with a nonchlorinated dibenzo-p-dioxin. <i>Physical Review B</i> , 2000, 61, 4425-4428.	1.1	0
804	Global warming potential assessment for CF ₃ OCF = CF ₂ . <i>Journal of Geophysical Research</i> , 2000, 105, 4019-4029.	3.3	24

#	ARTICLE	IF	CITATIONS
805	Functionalization of Diamond(100) by Cycloaddition of Butadiene: A First-Principles Theory. Journal of the American Chemical Society, 2000, 122, 12334-12339.	6.6	41
806	Theoretical Study of the Double Proton Transfer in the $\text{CH}_2\text{X}^+\text{XH}^-\text{X}^-\text{CH}_2\text{X}^+\text{XH}$ (X = O, S) Complexes. Journal of Physical Chemistry A, 2000, 104, 995-1003.	1.1	114
807	The Mechanism for Unimolecular Decomposition of RDX (1,3,5-Trinitro-1,3,5-triazine), an ab Initio Study. Journal of Physical Chemistry A, 2000, 104, 2261-2272.	1.1	241
808	Facial Selectivity in Epoxidation of 2-Cyclohexen-1-ol with Peroxy Acids. A Computational DFT Study. Journal of Organic Chemistry, 2000, 65, 8948-8959.	1.7	34
809	Homonuclear 3d transition-metal diatomics: A systematic density functional theory study. Journal of Chemical Physics, 2000, 113, 690-700.	1.2	249
810	Structure and vibrational spectra of $\text{H}^+(\text{H}_2\text{O})_8$: Is the excess proton in a symmetrical hydrogen bond?. Journal of Chemical Physics, 2000, 113, 5321.	1.2	47
811	Rearrangements of 2-Nitrobenzyl Compounds. 1. Potential Energy Surface of 2-Nitrotoluene and Its Isomers Explored with ab Initio and Density Functional Theory Methods. Journal of Physical Chemistry A, 2000, 104, 7856-7870.	1.1	75
812	Hydrogen Atom Adducts to Nitrobenzene: Formation of the Phenylnitronic Radical in the Gas Phase and Energetics of Wheland Intermediates. Journal of the American Chemical Society, 2000, 122, 9511-9524.	6.6	62
813	Activation of Small Alkanes in Ga-Exchanged Zeolites: A Quantum Chemical Study of Ethane Dehydrogenation. Journal of Physical Chemistry A, 2000, 104, 2468-2475.	1.1	82
814	Activation of ethane in Zn-exchanged zeolites: a theoretical study. Physical Chemistry Chemical Physics, 2000, 2, 1085-1089.	1.3	80
815	Mechanisms for the Adsorption of Substituted Nitrobenzenes by Smectite Clays. Environmental Science & Technology, 2001, 35, 4227-4234.	4.6	262
816	Ionized Phenol and Its Isomers in the Gas Phase. Journal of Physical Chemistry A, 2001, 105, 11582-11592.	1.1	51
817	Nonstoichiometric Defects and Optical Properties in LiNbO_3 . Journal of Physical Chemistry B, 2001, 105, 12242-12248.	1.2	71
818	Intrinsic and Environmental Effects on the Kinetic and Thermodynamics of Linkage Isomerization in Nitropentaamminecobalt(III) Complex. Journal of Physical Chemistry A, 2001, 105, 1086-1092.	1.1	23
819	Assessment of W1 and W2 theories for the computation of electron affinities, ionization potentials, heats of formation, and proton affinities. Journal of Chemical Physics, 2001, 114, 6014-6029.	1.2	444
820	Corannulene as a Lewis Base: Computational Modeling of Protonation and Lithium Cation Binding. Journal of the American Chemical Society, 2001, 123, 6687-6695.	6.6	67
821	Neural-network analysis of the vibrational spectra of N-acetyl-L-alanyl-L-methyl amide conformational states. Physical Review E, 2001, 64, 021905.	0.8	18
822	Mechanism for Unimolecular Decomposition of HMX (1,3,5,7-Tetranitro-1,3,5,7-tetrazocine), an ab Initio Study. Journal of Physical Chemistry A, 2001, 105, 1302-1314.	1.1	152

#	ARTICLE	IF	CITATIONS
823	Theoretical studies of diiron(II) complexes that model features of the dioxygen-activating centers in non-heme diiron enzymes. <i>Israel Journal of Chemistry</i> , 2001, 41, 173-186.	1.0	9
824	Ab Initio Investigation of Physisorption of Molecular Hydrogen on Planar and Curved Graphenes. <i>Journal of Physical Chemistry B</i> , 2001, 105, 3470-3474.	1.2	282
825	New Sorbents for Desulfurization of Liquid Fuels by π -Complexation. <i>Industrial & Engineering Chemistry Research</i> , 2001, 40, 6236-6239.	1.8	165
826	Revisiting Markovnikov Addition to Alkenes via Molecular Electrostatic Potential. <i>Journal of Organic Chemistry</i> , 2001, 66, 6883-6890.	1.7	66
827	An ab Initio Theory and Density Functional Theory (DFT) Study of Conformers of Tetrahydro-2H-pyran. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10123-10132.	1.1	33
828	Prediction of transition state barriers and enthalpies of reaction by a new hybrid density-functional approximation. <i>Journal of Chemical Physics</i> , 2001, 115, 11040-11051.	1.2	177
829	Kinetics and Mechanism of the Reactions of Ground-State Y (4d15s2,2D) with Ethylene and Propylene: \hat{A} Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6655-6667.	1.1	88
830	Electron Affinities of Polycyclic Aromatic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2001, 105, 524-528.	1.1	124
831	Modeling the Active Sites of Metalloenzymes. 4. Predictions of the Unready States of [NiFe]Desulfovibrio gigas Hydrogenase from Density Functional Theory. <i>Inorganic Chemistry</i> , 2001, 40, 18-24.	1.9	61
832	Electron transfer in a trinuclear oxo-centred mixed-valence iron complex, in solid and solution states Dedicated to Professor Dieter Sellmann on the occasion of his 60th birthday.. <i>Dalton Transactions RSC</i> , 2001, , 3373-3383.	2.3	47
833	Charge transfer and σ -band lineup in molecular electronic devices: A chemical and numerical interpretation. <i>Journal of Chemical Physics</i> , 2001, 115, 4292-4299.	1.2	471
834	A Density Functional Study of EPR Parameters for Vanadyl Complexes Containing Schiff Base Ligands. <i>Journal of Physical Chemistry B</i> , 2001, 105, 12644-12652.	1.2	67
835	Glyoxal photodissociation. An ab initio direct classical trajectory study of $C_2H_2O_2^+ + H_2 \rightarrow \hat{A} CO$. <i>Journal of Chemical Physics</i> , 2001, 114, 8897-8904.	1.2	34
836	Enhanced Stability of Non-Proton-Transferred Clusters of Hydrated Hydrogen Fluoride $HF(H_2O)_n$ ($n = 1-10$). <i>Journal of Physical Chemistry B</i> , 2001, 105, 12644-12652.	1.1	43
837	Large-Scale ab Initio Quantum Chemical Calculations on Biological Systems. <i>Accounts of Chemical Research</i> , 2001, 34, 351-358.	7.6	101
838	ONIOM Study of Chemical Reactions in Microsolvation Clusters: $(H_2O)_n CH_3Cl + OH \cdot (H_2O)_m$ ($n+m=1-10$). <i>Journal of Physical Chemistry B</i> , 2001, 105, 12644-12652.	1.1	43
839	Structure and dynamics of triethylamine and tripropylamine radical cations generated in AlPO ₄ -5 by ionizing radiation: an EPR and MO study. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 1611-1616.	1.3	22
840	The structure and electronic properties of silicon oxynitride gate dielectrics. <i>Semiconductor Science and Technology</i> , 2001, 16, 467-470.	1.0	20

#	ARTICLE	IF	CITATIONS
841	Density functional theory: coverage of dynamic and non-dynamic electron correlation effects. <i>Molecular Physics</i> , 2001, 99, 1899-1940.	0.8	281
842	Ferroelectric Liquid Crystals Induced by Atropisomeric Biphenyl Dopants: Dependence of the Polarization Power on the Nature of the Symmetry-Breaking Groups. <i>Chemistry of Materials</i> , 2001, 13, 1692-1699.	3.2	26
843	Electronic Structure of 3d [M(H ₂ O) ₆] ³⁺ Ions from Sc III to Fe II: A Quantum Mechanical Study Based on DFT Computations and Natural Bond Orbital Analyses. <i>Inorganic Chemistry</i> , 2001, 40, 3101-3112.	1.9	55
844	Electron localization function studies of the nature of binding in neutral rare-gas containing hydrides: HKrCN, HKrNC, HXeCN, HXeNC, HXeOH, and HXeSH. <i>Journal of Chemical Physics</i> , 2001, 114, 4349.	1.2	33
845	The Nature of Binding in HRgY Compounds (Rg = Ar, Kr, Xe; Y = F, Cl) Based on the Topological Analysis of the Electron Localisation Function (ELF). <i>Progress in Theoretical Chemistry and Physics</i> , 2001, , 259-279.	0.2	11
846	Pressure-temperature anomalies of doped ZnO polycrystalline films deposited on bare glasses. <i>Materials Letters</i> , 2001, 51, 519-524.	1.3	11
847	Quantum Chemistry and Classical Simulations of Metal Complexes in Aqueous Solutions. <i>Reviews in Mineralogy and Geochemistry</i> , 2001, 42, 273-317.	2.2	15
848	Coordination Sphere Flexibility of Active-Site Models for Fe-Only Hydrogenase: Studies in Intra- and Intermolecular Diatomic Ligand Exchange. <i>Journal of the American Chemical Society</i> , 2001, 123, 3268-3278.	6.6	283
849	Combined Pseudopotential and Density Functional Study of Bis- η^6 -benzene d and f Element Complexes. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 18-21.	2.8	30
850	Nitrobenzene Isomers. <i>Journal of Physical Chemistry A</i> , 2001, 105, 995-1010.	1.1	20
851	Theoretical study of the hydrogen abstraction reactions for CH ₃ R + Cl \rightarrow CH ₂ R + HCl (R = Cl and Br). <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 3955-3960.	1.3	18
852	Oxidation of palladium powder by the adduct Ph ₂ P(S)NHP(S)Ph ₂ . Crystal structure of PdL ₂ . <i>Dalton Transactions RSC</i> , 2001, , 1105-1110.	2.3	19
853	Simple analysis of intermolecular potentials—the mBq pair potential for collisions and energy transfer. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 2209-2215.	1.3	4
854	Electron affinities of cyano-substituted ethylenes. <i>Molecular Physics</i> , 2001, 99, 663-675.	0.8	13
855	Orbital energy analysis with respect to LDA and self-interaction corrected exchange-only potentials. <i>Journal of Chemical Physics</i> , 2001, 114, 639.	1.2	63
856	Structure of alkali tellurite glasses from neutron diffraction and molecular orbital calculations. <i>Journal of Chemical Physics</i> , 2001, 114, 459.	1.2	37
857	An experimental and theoretical approach to phosphonodithioato complexes: molecular orbital analysis by hybrid-DFT and EHT calculations on trans-bis[O-alkyl-phenylphosphonodithioato]NiII, and vibrational assignments. <i>Canadian Journal of Chemistry</i> , 2001, 79, 1483-1491.	0.6	17
858	Molecular dynamics simulations of plastoquinone in solution. <i>Molecular Physics</i> , 2001, 99, 247-253.	0.8	16

#	ARTICLE	IF	CITATIONS
859	Carbohydrate-derived dienes for intramolecular and asymmetric Diels-Alder reactions. <i>Journal of the Chemical Society, Perkin Transactions 1</i> , 2001, , 754-762.	1.3	10
860	Does the cationic or the radical character dominate the reactivity of alkene radical cations towards solvent molecules?. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 1246-1252.	1.3	10
861	Theoretical study on the atmospheric fate of carbonyl radicals: kinetics of decomposition reactions. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 4712.	1.3	58
862	Interplay of Intrinsic and Environmental Effects on the Magnetic Properties of Free Radicals Issuing from H-Atom Addition to Cytosine. <i>Journal of the American Chemical Society</i> , 2001, 123, 7113-7117.	6.6	22
863	A more efficient copper-ion-exchanged ZSM-5 zeolite for N ₂ adsorption at room temperature: Ion-exchange in an aqueous solution of Cu(CH ₃ COO) ₂ . <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 1383-1390.	1.3	46
864	Palladium-catalysed oxidation of alcohols to carbonyl compounds with 1,2-dichloroethane as the primary oxidant: a theoretical study. Electronic supplementary information (ESI) available: Tables of absolute energies and structural parameters for all of the computed species. See http://www.rsc.org/suppdata/p2/b1/b102256n/ . <i>Perkin Transactions II RSC</i> , 2001, , 1998-2004.	1.1	1
865	On the regioselectivity of nucleophilic additions to anisole-Cr(CO) ₃ and related complexes: a density functional study. <i>New Journal of Chemistry</i> , 2001, 25, 446-450.	1.4	16
866	A Theoretical Study of the Gas-Phase Pyrolysis of 2-Azidoacetic Acid. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3140-3147.	1.1	18
867	Theoretical Investigation of Steric and Electronic Effects in Coenzyme B ₁₂ Models. <i>Organometallics</i> , 2001, 20, 550-556.	1.1	58
868	Ionized Benzonitrile and Its Distonic Isomers in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8579-8587.	1.1	23
869	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 18. Catalytic Transfer Dehydrogenation of Alkanes by an Iridium(III) Pincer Complex. <i>Organometallics</i> , 2001, 20, 2153-2160.	1.1	38
870	Theoretical Study on the Low-Energy and High-Energy Conformers of the Three Isomers of 1,4-Difluorobutadiene. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10372-10378.	1.1	9
871	Mechanism of electron trapping in Ge-doped SiO ₂ glass. <i>Applied Physics Letters</i> , 2001, 79, 359-361.	1.5	10
872	Modeling the Active Sites in Metalloenzymes 5. The Heterolytic Bond Cleavage of H ₂ in the [NiFe] Hydrogenase of <i>Desulfovibrio gigas</i> by a Nucleophilic Addition Mechanism. <i>Inorganic Chemistry</i> , 2001, 40, 6201-6203.	1.9	61
873	Absolute Configuration and Conformational Stability of (+)-2,5-Dimethylthiolane and (âˆ-)2,5-Dimethylsulfolane. <i>Journal of Organic Chemistry</i> , 2001, 66, 3507-3512.	1.7	14
874	CS ₂ Fixation by Carbonic Anhydrase Model Systems A New Substrate in the Catalytic Cycle. <i>Inorganic Chemistry</i> , 2001, 40, 1006-1013.	1.9	23
875	Catalytic Mechanism of Glyoxalase I: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 10280-10289.	6.6	50
876	Theoretical Study on the Potential Energy Surface of the 1CH ₂ +N ₂ O Reaction. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5885-5895.	1.1	7

#	ARTICLE	IF	CITATIONS
877	A Density Functional Study on the Effect of the Trans Axial Ligand of Cobalamin on the Homolytic Cleavage of the Co-C Bond. <i>Journal of Physical Chemistry B</i> , 2001, 105, 7564-7571.	1.2	74
878	Reactivity of phosphonodithioato Ni(II) complexes: solution equilibria, solid state studies and theoretical calculations on the adduct formation with some pyridine derivatives. <i>Dalton Transactions RSC</i> , 2001, , 2671-2677.	2.3	46
879	Structure, Torsional Potentials, and Thermodynamic Properties of $\text{CH}_2\text{ClOCH}_3$, $\text{CHCl}_2\text{OCH}_3$, and CCl_3OCH_3 . Density Functional and ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5420-5430.	1.1	8
880	Cycloaddition of Carbonyl Compounds on Si(100): A New Mechanisms and Approaches to Selectivity for Surface Cycloaddition Reactions. <i>Journal of the American Chemical Society</i> , 2001, 123, 7340-7346.	6.6	58
881	Modeling the Action of an Antitumor Drug: A Density Functional Theory Study of the Mechanism of Tirapazamine. <i>Journal of the American Chemical Society</i> , 2001, 123, 7320-7325.	6.6	23
882	Absorption and Fluorescence Excitation Spectra of 9-(N-carbazolyl)-anthracene: Effects of Intramolecular Vibrational Redistribution and Diabatic Transitions Involving Electron Transfer. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2911-2924.	1.1	17
883	Hydrogen-Bond Mediated Catalysis: The Aminolysis of 6-Chloropyrimidine as Catalyzed by Derivatives of Uracil. <i>Journal of the American Chemical Society</i> , 2001, 123, 2047-2052.	6.6	8
884	Is the Bis- μ -Oxo $\text{Cu}_2(\text{III},\text{III})$ State an Intermediate in Tyrosinase?. <i>Journal of the American Chemical Society</i> , 2001, 123, 11819-11820.	6.6	61
885	Anion Photoelectron Spectroscopy of Aluminum Phosphide Clusters. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6886-6893.	1.1	78
886	A quantum chemistry approach for current-voltage characterization of molecular junctions. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 5017-5023.	1.3	95
887	Three Conformational Polymorphs of Di- μ -chlorotetrakis(1-methylboratabenzene)diyttrium: Synthesis, X-ray Structures, Quantum Chemical Calculations, and Lattice Energy Minimizations. <i>Inorganic Chemistry</i> , 2001, 40, 3117-3123.	1.9	27
888	A Jahn-Teller Geometric Distortion Effect on the Woodward-Hoffmann Rule in Thermal Decompositions of Diazetines. <i>Journal of Physical Chemistry A</i> , 2001, 105, 7281-7286.	1.1	10
889	Description of $\text{C}(\text{sp}^2)\text{-C}(\text{sp}^2)$ Rotation in Butadiene by Density Functionals. <i>Journal of Physical Chemistry A</i> , 2001, 105, 11541-11548.	1.1	34
890	Singlet and Triplet Reaction Paths for Gas-Phase $\text{Zr} + \text{C}_2\text{H}_4$ by Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4851-4864.	1.1	83
891	Migration Tendencies of Group 14 Element Ligands in the Coordination Sphere of Cationic Phosphonium Iron Complexes. <i>Organometallics</i> , 2001, 20, 4333-4344.	1.1	16
892	Black Body Fragmentation of Cationic Ammonia Clusters. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6386-6392.	1.1	71
893	A theoretical study of the polarized neutron scattering from Cs_3CoCl_5 . <i>Journal of Chemical Physics</i> , 2001, 114, 2687-2697.	1.2	6
894	Large Enhancement of Reactivity of Diels-Alder Reactions on a $\text{C}(001)(2 \times 1)$ Surface: A Hybrid Density-Functional Study. <i>Journal of Physical Chemistry B</i> , 2001, 105, 1813-1816.	1.2	23

#	ARTICLE	IF	CITATIONS
895	Electron Affinities of the DNA and RNA Bases. <i>Journal of the American Chemical Society</i> , 2001, 123, 4023-4028.	6.6	236
896	An Isomer Prediction Model for PCNs, PCDD/Fs, and PCBs from Municipal Waste Incinerators. <i>Environmental Science & Technology</i> , 2001, 35, 3175-3181.	4.6	46
897	Allylic Alcohol Epoxidation by Methyltrioxorhenium: A Density Functional Study on the Mechanism and the Role of Hydrogen Bonding. <i>Journal of the American Chemical Society</i> , 2001, 123, 2365-2376.	6.6	49
898	Benchmark ab Initio Energy Profiles for the Gas-Phase SN2 Reactions $Y^- + CH_3X \rightarrow CH_3Y + X^-$ (X, Y = F, Cl, Br). Validation of Hybrid DFT Methods. <i>Journal of Physical Chemistry A</i> , 2001, 105, 895-904.	1.1	199
899	Electronic Spectra of 2,2'-Bithiophene and 2,2':5,2''-Terthiophene Radical Cations: A Theoretical Analysis. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9788-9794.	1.1	22
900	Absolute Configurations, Predominant Conformations, and Tautomeric Structures of Enantiomeric tert-Butylphenylphosphinothioic Acid. <i>Journal of Organic Chemistry</i> , 2001, 66, 9015-9019.	1.7	20
901	A Consistent Approach toward Atomic Radii. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5940-5944.	1.1	66
902	Spectroscopic Properties and Electronic Structure of Low-Spin Fe(III) Alkylperoxo Complexes: Homolytic Cleavage of the O-O Bond. <i>Journal of the American Chemical Society</i> , 2001, 123, 8271-8290.	6.6	132
903	Quantum Chemical Studies of Carbohydrate Reactivity: Acid Catalyzed Ring Opening Reactions. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8216-8222.	1.1	15
904	Possible Dissociative Adsorption of CH ₃ OH and CH ₃ NH ₂ on Si(100)-2 × 1 Surface. <i>Journal of Physical Chemistry B</i> , 2001, 105, 10340-10347.	1.2	78
905	Molecular dynamics simulations of ubiquinone; a survey over torsional potentials and hydrogen bonds. <i>Molecular Physics</i> , 2001, 99, 1795-1804.	0.8	15
906	A Density Functional Theory Study on the Mechanism of the Permanganate Oxidation of Substituted Alkenes. <i>Journal of Organic Chemistry</i> , 2001, 66, 672-676.	1.7	41
907	Stereoelectronic Effects in the Si-C Bond: A Study of the Molecular Structure and Conformation of Tetraphenylsilane by Gas-Phase Electron Diffraction and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5933-5939.	1.1	16
908	Catalytic Roles of Copper on Chlorination of Precursor Phenol for Dioxins Using Ab Initio Molecular Orbital Method. <i>Materials Transactions</i> , 2001, 42, 2537-2542.	0.4	3
909	Interpretation and Calculation of Spin-Hamiltonian Parameters in Transition Metal Complexes. , 0, , 345-466.		5
910	Catalytic Reactions of Radical Enzymes. <i>Theoretical and Computational Chemistry</i> , 2001, 9, 145-181.	0.2	0
911	A multi-component model for radiation damage to DNA from its constituents. <i>Theoretical and Computational Chemistry</i> , 2001, 9, 409-466.	0.2	5
912	Reparameterization of hybrid functionals based on energy differences of states of different multiplicity. <i>Theoretical Chemistry Accounts</i> , 2001, 107, 48-55.	0.5	1,240

#	ARTICLE	IF	CITATIONS
913	Theoretical evaluation of the hydrogen kinetic isotope effect on the first step of the methylmalonyl-CoA mutase reaction. <i>Journal of Inorganic Biochemistry</i> , 2001, 86, 681-689.	1.5	26
914	Theoretical studies on magnetic interactions of the metal dimers and their acetate complexes. <i>Polyhedron</i> , 2001, 20, 1189-1196.	1.0	20
915	A density functional approach of prototropic tautomerism of guanine. <i>Chemical Physics</i> , 2001, 264, 187-196.	0.9	26
916	A density functional theory investigation of CrSin (n=1-6) clusters. <i>Chemical Physics</i> , 2001, 263, 255-262.	0.9	94
917	The photophysics of pyranthione: a theoretical investigation focussing on spin-forbidden transitions. <i>Chemical Physics</i> , 2001, 264, 245-254.	0.9	23
918	Crystallographic and theoretical investigations of the preferred conformations of three isomeric N-acetyl-dihydro-oxadiazoles. <i>Journal of Molecular Structure</i> , 2001, 561, 29-41.	1.8	3
919	Photoelectron spectra and electronic structures of highly substituted polyenes. <i>Journal of Molecular Structure</i> , 2001, 567-568, 11-18.	1.8	8
920	Two possible reaction pathways for the formation of a ruthenium carbene complex by addition of acetylene to [RuH ₂ Cl ₂ (PH ₃) ₂]: a quantum chemical study. <i>Journal of Organometallic Chemistry</i> , 2001, 617-618, 225-232.	0.8	12
921	Implication of palladium geometric and electronic structures to hydrogen activation on bulk surfaces and clusters. <i>Journal of Molecular Catalysis A</i> , 2001, 173, 19-59.	4.8	71
922	Infrared and Raman spectroscopy of 9-acridinones. <i>Vibrational Spectroscopy</i> , 2001, 27, 139-152.	1.2	7
923	IR study of the N,N'-triphenylguanidine and its imine nitrogen coordinated Pd(II) complexes. <i>Vibrational Spectroscopy</i> , 2001, 27, 153-164.	1.2	14
924	Fourier transform infrared and Raman spectra, vibrational assignment and ab initio calculations of terephthalic acid and related compounds. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2001, 57, 993-1007.	2.0	121
925	Density functional theory study of the Fourier transform infrared and Raman spectra of dichloro-bis(2,4-pentanedionate)tin(IV). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2001, 57, 1149-1161.	2.0	10
926	Structural chemistry of polycyclic heteroaromatic compounds. Part 13. Photoelectron spectra and electronic structures of tricyclic heteroarenes of the anthracene type. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2001, 57, 2475-2483.	2.0	4
927	Electron energy loss and dissociative electron attachment spectroscopy of methyl vinyl ether and related compounds. <i>International Journal of Mass Spectrometry</i> , 2001, 205, 43-55.	0.7	15
928	Nitrobenzene as a material for the fast-response degenerate four-wave mixing. <i>Optical Materials</i> , 2001, 16, 417-429.	1.7	22
929	Tautomerism in 4-substituted 1-phenyl-3-methyl-pyrazolin-5-ones-a theoretical and ¹³ C NMR study. <i>Journal of Physical Organic Chemistry</i> , 2001, 14, 566-576.	0.9	34
930	Predominance of 2-arylhydrazones of 1,3-diphenylpropane-1,2,3-trione over its proton-transfer products. <i>Journal of Physical Organic Chemistry</i> , 2001, 14, 797-803.	0.9	13

#	ARTICLE	IF	CITATIONS
931	B3LYP studies of the formation of neutral tyrosyl radical Yz [•] and regeneration of neutral tyrosine Yz in PSII. <i>International Journal of Quantum Chemistry</i> , 2001, 83, 220-229.	1.0	15
932	Influence of the alkyl chain length on the excited-state properties of 4-dialkyl-benzonitriles. A theoretical DFT/MRCI study. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 149-156.	1.0	10
933	Improvement of the hybrid density functional method from the viewpoint of effective exchange integrals. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 592-600.	1.0	36
934	Fourier transform infrared study on the sorption of water to various kinds of polymer thin films. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2001, 39, 2175-2182.	2.4	65
935	DFT/MRCI calculations on the excited states of porphyrin, hydroporphyrins, tetrazaporphyrins and metalloporphyrins. <i>Journal of Porphyrins and Phthalocyanines</i> , 2001, 05, 225-232.	0.4	100
936	GIAO/DFT calculated chemical shifts of tautomeric species. 2-Phenacylpyridines and (Z)-2-(2-hydroxy-2-phenylvinyl)pyridines. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, 334-340.	1.1	166
937	Theoretical study of the mechanism of peptide ring formation in green fluorescent protein. <i>International Journal of Quantum Chemistry</i> , 2001, 81, 169-186.	1.0	30
938	Distorted silicon hydrides? a comparative study with various density functionals. <i>Journal of Computational Chemistry</i> , 2001, 22, 151-161.	1.5	12
939	Chemistry with ADF. <i>Journal of Computational Chemistry</i> , 2001, 22, 931-967.	1.5	8,854
940	OH hydrogen abstraction reactions from alanine and glycine: A quantum mechanical approach. <i>Journal of Computational Chemistry</i> , 2001, 22, 1138-1153.	1.5	57
941	Theoretical prediction of vertical transition energies of diaminosilylenes and aminosubstituted disilenes. <i>Journal of Computational Chemistry</i> , 2001, 22, 1536-1541.	1.5	23
942	A density functional theory study of the dimers of HX (X = F, Cl, and Br). <i>Journal of Computational Chemistry</i> , 2001, 22, 1590-1597.	1.5	26
943	Modeling aspects of mechanisms for reactions catalyzed by metalloenzymes. <i>Journal of Computational Chemistry</i> , 2001, 22, 1634-1645.	1.5	127
944	Parametrization of the Becke3-LYP hybrid functional for a series of small molecules using quantum molecular similarity techniques. <i>Journal of Computational Chemistry</i> , 2001, 22, 1666-1678.	1.5	21
945	Photoelectron Spectra, Electronic Structures, and Conformational Properties of (E)-Stilbene, Styrylthiophenes, and (Thienylethenyl)pyridines. <i>European Journal of Organic Chemistry</i> , 2001, 2001, 121-130.	1.2	16
950	Three- and Four-Membered Rings from Cycloadditions of 1,3-Thiazolium-4-olates and Aldehydes. <i>Chemistry - A European Journal</i> , 2001, 7, 3033-3042.	1.7	17
951	Mechanistic Aspects of the Reaction between Br ₂ and Chalcogenone Donors (LE; E=S, Se): Competitive Formation of 10-E-3, T-Shaped 1:1 Molecular Adducts, Charge-Transfer Adducts, and [(LE) ₂] ²⁺ Dications. <i>Chemistry - A European Journal</i> , 2001, 7, 3122-3133.	1.7	68
952	Nonorthogonal Dilithium-1,3-biborataallenes Containing Planar-Tetracoordinate Carbon Atoms. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 2662-2665.	7.2	24

#	ARTICLE	IF	CITATIONS
953	Carbanions Substituted by Transition Metals: Synthesis, Structure, and Configurational Restrictions of a Lithium Titanium Phosphonate. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 2890-2893.	7.2	20
954	1,2-Bis(3-methyl-imidazolin-2-ylum iodobromoselenanide)ethane: Oxidative Addition of IBr at the Se Atom of a >C=Se Group. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 4229-4232.	7.2	50
955	Theoretical Elucidation of Structure-Antioxidant Activity Relationships for Thiazolidinone Derivatives. <i>QSAR and Combinatorial Science</i> , 2001, 20, 139-142.	1.4	11
956	O-H Bond Dissociation Energies of Phenolic Compounds are Determined by Field/Inductive Effect or Resonance Effect? A DFT Study and Its Implication. <i>QSAR and Combinatorial Science</i> , 2001, 20, 148-152.	1.4	49
957	Automatic code generation in density functional theory. <i>Computer Physics Communications</i> , 2001, 136, 310-318.	3.0	27
958	First principles simulation of surfaces and interfaces. <i>Computer Physics Communications</i> , 2001, 137, 59-73.	3.0	9
959	Density matrix functional theory in average and relative coordinates. <i>Chemical Physics Letters</i> , 2001, 335, 409-419.	1.2	5
960	Assessment of a new local exchange functional OPTX. <i>Chemical Physics Letters</i> , 2001, 341, 319-328.	1.2	472
961	Electronic spectroscopy of organic acid dimers. <i>Chemical Physics Letters</i> , 2001, 343, 159-165.	1.2	30
962	A computational study of the mechanism for self-assembly of N-pyrrolyl radicals on Si(1 0 0)-2Å-1. <i>Chemical Physics Letters</i> , 2001, 343, 219-224.	1.2	27
963	Transient resonance Raman and density functional theory investigation of CH ₃ I produced from ultraviolet photolysis of iodomethane in the solution phase. <i>Chemical Physics Letters</i> , 2001, 349, 291-298.	1.2	7
964	Transient resonance Raman and density functional theory investigation of the ultraviolet photolysis of dibromoacetonitrile in the solution phase. <i>Chemical Physics Letters</i> , 2001, 350, 78-85.	1.2	0
965	Nitromethyl Radical, Cation, and Anion. A Neutralization and Electron Photodetachment Reionization Mass Spectrometric and ab Initio Computational Study of [C,H ₂ ,N,O ₂] Isomers. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1371-1382.	1.1	15
966	Molecular tests of the random phase approximation to the exchange-correlation energy functional. <i>Physical Review B</i> , 2001, 64, .	1.1	400
967	Ab Initio Investigation of Hydrogenation of C ₆₀ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 7634-7637.	1.1	28
968	Title is missing!. <i>Russian Chemical Bulletin</i> , 2001, 50, 2064-2070.	0.4	13
969	Origin of Nonlinear Optical Susceptibility in SiC Nanocrystallites. <i>Journal of Cluster Science</i> , 2001, 12, 399-419.	1.7	20
970	Title is missing!. <i>Russian Journal of Electrochemistry</i> , 2001, 37, 15-25.	0.3	8

#	ARTICLE	IF	CITATIONS
971	Effect of medium on the rate constant of decarbonylation of phenylacetyl radical. Russian Chemical Bulletin, 2001, 50, 237-240.	0.4	5
972	Title is missing!. Kinetics and Catalysis, 2001, 42, 404-410.	0.3	2
973	Quantum-Chemical Study of Alkyl Carbenium Ions in 100% Sulfuric Acid. Kinetics and Catalysis, 2001, 42, 411-417.	0.3	4
974	Title is missing!. Russian Journal of General Chemistry, 2001, 71, 780-785.	0.3	0
975	Reversible Carbon-Carbon Double Bond Cleavage of a Ketene Ligand at a Single Iridium(I) Center: A Theoretical Study. Organometallics, 2001, 20, 3938-3949.	1.1	45
976	Photoinduced non-linear optical diagnostic of SiNxOy/SiO2 interfaces. Optics and Lasers in Engineering, 2001, 35, 239-250.	2.0	14
977	Excited state intramolecular charge transfer in N,N-heterocyclic-4-aminobenzonitriles: a DFT study. Chemical Physics Letters, 2001, 340, 531-537.	1.2	25
978	Electronic and structural effects determining rotational barriers about the C-N bond in enamines of pyran-4-one and thiopyran-4-one. A theoretical MO ab initio approach to the interpretation of experimental results. Computational and Theoretical Chemistry, 2001, 535, 257-267.	1.5	6
979	Nitrogen-inversion in some aziridine type compounds: structural and kinetic investigations by ab initio methods. Computational and Theoretical Chemistry, 2001, 535, 247-256.	1.5	11
980	Is HCCP linear, bent or cyclic? Structures and energies of its low-lying states. Computational and Theoretical Chemistry, 2001, 536, 123-132.	1.5	7
981	Thermochemical analysis of the OH+C2H4+C2H4OH reaction using accurate theoretical methods. Computational and Theoretical Chemistry, 2001, 537, 199-212.	1.5	17
982	Theoretical analysis of the energy levels induced by oxygen vacancies and the doping process (Co, Cu) in ZnO. Journal of Applied Physics, 2001, 91, 7843-7851.	1.5	21
983	Study of the electronic structure of molecules. XXIII. Decomposition of correlation energy into atomic, covalent, ionic and van der Waals components. Computational and Theoretical Chemistry, 2001, 543, 39-52.	1.5	5
984	A density functional investigation of MoSin (n=1-6) clusters. Computational and Theoretical Chemistry, 2001, 549, 165-180.	1.5	61
985	Comparative study of the molecular structure of stilbene using molecular mechanics, Hartree-Fock and density functional theories. Computational and Theoretical Chemistry, 2001, 549, 63-67.	1.5	15
986	A theoretical study of the anionic intermolecular hydrogen bonding between dihydroxy tetrahydrofuran and phosphate ions. Computational and Theoretical Chemistry, 2001, 574, 75-83.	1.5	9
987	The rovibrational structure of the He-CO complex from a model interaction potential. Molecular Physics, 2001, 99, 689-698.	0.8	21
988	Catalytic effects of copper on dibenzo-p-dioxin and polychlorinated dibenzo-p-dioxin generations using ab initio molecular orbital method. Toxicological and Environmental Chemistry, 2001, 81, 133-146.	0.6	4

#	ARTICLE	IF	CITATIONS
989	Density Functional Theory, Methods, Techniques, and Applications. , 2001, , 105-160.		1
991	New computational strategies for the quantum mechanical study of biological systems in condensed phases. Theoretical and Computational Chemistry, 2001, , 467-538.	0.2	18
992	Generation of Free Radicals by Emodic Acid and its [d-Lys6]GnRH-conjugate. Photochemistry and Photobiology, 2001, 74, 226.	1.3	24
993	Structures, thermochemistry, and electron affinities of the disilicon fluorides, Si ₂ F _n /Si ₂ F _n ⁻ (n= 1-6). Molecular Physics, 2001, 99, 1053-1074.	0.8	14
994	Comparative study of density-functional theories of the exchange-correlation hole and energy in silicon. Physical Review B, 2001, 64, .	1.1	14
995	Transition state dynamics of the OH+OH ⁺ O+H ₂ O reaction studied by dissociative photodetachment of H ₂ O ⁺ . Journal of Chemical Physics, 2001, 115, 6931-6940.	1.2	25
996	The performance of density functional theory for equilibrium molecular properties of symmetry breaking molecules. Journal of Chemical Physics, 2001, 114, 8257-8269.	1.2	39
997	Rotational dynamics of coumarins: An experimental test of dielectric friction theories. Journal of Chemical Physics, 2001, 114, 6702-6713.	1.2	70
998	Photodissociation of acetaldehyde: The CH ₄ +CO channel. Journal of Chemical Physics, 2001, 114, 6128-6133.	1.2	52
999	Transient resonance Raman spectroscopy and density functional theory investigation of iso-CHBr ₂ Cl and iso-CCl ₃ Br photoproducts produced following ultraviolet excitation of CHBr ₂ Cl and CCl ₃ Br. Journal of Chemical Physics, 2001, 114, 8347-8356.	1.2	34
1000	Rotational dynamics of coumarins in nonassociative solvents: Point dipole versus extended charge distribution models of dielectric friction. Journal of Chemical Physics, 2001, 115, 4732-4741.	1.2	37
1001	Symmetry-breaking and near-symmetry-breaking in three-electron-bonded radical cations. Journal of Chemical Physics, 2001, 115, 90-102.	1.2	37
1002	Cycloaddition reaction of furan with Si(100)-2 \times 1. Journal of Chemical Physics, 2001, 114, 2766-2774.	1.2	33
1003	Infrared and density-functional-theory study of spherosiloxane-based model silicon/silicon oxide interfaces. Physical Review B, 2001, 64, .	1.1	11
1004	Ab initio study of the initial growth mechanism of silicon nitride on Si(100)-2 \times 1 using NH ₃ . Physical Review B, 2001, 64, .	1.1	49
1005	Density functional theory predictions of anharmonicity and spectroscopic constants for diatomic molecules. Journal of Chemical Physics, 2001, 115, 2439-2448.	1.2	39
1006	Band structure treatment of the influence of nonstoichiometric defects on optical properties in LiNbO ₃ . Journal of Applied Physics, 2001, 90, 5542-5549.	1.1	99
1007	Comparison of ab initio and density functional calculations of electric field gradients: The ⁵⁷ Fe nuclear quadrupole moment from M \ddot{u} ssbauer data. Journal of Chemical Physics, 2001, 115, 5913-5924.	1.2	47

#	ARTICLE	IF	CITATIONS
1008	The rovibrational structure of the Ar ⁺ CO complex from a model interaction potential. <i>Journal of Chemical Physics</i> , 2001, 115, 249-256.	1.2	23
1009	Photoelectron spectroscopy of GaX ₂ ⁺ , Ga ₂ X ⁺ , Ga ₂ X ₂ ⁺ , and Ga ₂ X ₃ ⁺ (X=P,As). <i>Journal of Chemical Physics</i> , 2001, 115, 4620-4631.	1.2	64
1010	New correlation energy functionals with explicit dependence on the number of electrons. <i>Journal of Chemical Physics</i> , 2002, 116, 10571-10576.	1.2	4
1011	Quantum chemical study of the elementary reactions in zirconium oxide atomic layer deposition. <i>Applied Physics Letters</i> , 2002, 81, 304-306.	1.5	54
1012	Effective- J model Hamiltonian parameters of monolayered cuprate superconductors from ab initio electronic structure calculations. <i>Physical Review B</i> , 2002, 65, .	1.1	50
1013	Atomic layer deposition of hafnium oxide: A detailed reaction mechanism from first principles. <i>Journal of Chemical Physics</i> , 2002, 117, 1931-1934.	1.2	99
1014	Quantum chemical study of the mechanism of aluminum oxide atomic layer deposition. <i>Applied Physics Letters</i> , 2002, 80, 3304-3306.	1.5	178
1015	CF ₃ I on a silicon surface: Adsorption, temperature-programmed desorption, and electron-stimulated desorption. <i>Journal of Chemical Physics</i> , 2002, 116, 10402-10410.	1.2	6
1016	Electron attachment to SF ₅ CF ₃ (296–563 K) and calculations of the neutral and anion thermochemistry. <i>Journal of Chemical Physics</i> , 2002, 116, 6021-6027.	1.2	26
1017	Hydrogen adsorption on phosphorus-rich (2 $\bar{1}$) indium phosphide (001). <i>Physical Review B</i> , 2002, 65, .	1.1	29
1018	Density functional theory of spin-coupled models for diiron-oxo proteins: Effects of oxo and hydroxo bridging on geometry, electronic structure, and magnetism. <i>Journal of Chemical Physics</i> , 2002, 116, 6253-6270.	1.2	56
1019	Direct Method for Optimized Effective Potentials in Density-Functional Theory. <i>Physical Review Letters</i> , 2002, 89, 143002.	2.9	250
1020	Spectroscopy of the low-lying states of the group III ⁺ V diatomics, AlP, GaP, InP, and GaAs via anion photodetachment spectroscopy. <i>Journal of Chemical Physics</i> , 2002, 117, 8644-8656.	1.2	33
1021	Velocity map imaging of ion-molecule reaction products: Co ⁺ (3F ₄)+isobutane. <i>Journal of Chemical Physics</i> , 2002, 117, 653-665.	1.2	24
1022	Time-resolved resonance Raman spectroscopy and density functional theory investigation of the CH ₂ I ⁺ I isomer and CH ₂ I ₂ ⁺ molecular complex products produced from ultraviolet photolysis of CH ₂ I ₂ in the solution phase: Comparison of the structure and chemical reactivity of polyhalomethane isomers and polyhalomethane ⁺ halogen atom molecular complexes. <i>Journal of Chemical Physics</i> , 2002, 117, 7931-7941.	1.2	19
1023	One-color multiphoton threshold photoelectron spectra of methyl bromide, and their comparison with methyl iodide. <i>Journal of Chemical Physics</i> , 2002, 116, 4938.	1.2	33
1024	An accurate MGGA-based hybrid exchange-correlation functional. <i>Journal of Chemical Physics</i> , 2002, 116, 2335-2337.	1.2	20
1025	Effect of Fock exchange on the electronic structure and magnetic coupling in NiO. <i>Physical Review B</i> , 2002, 65, .	1.1	360

#	ARTICLE	IF	CITATIONS
1026	Scaling the spin densities separately in density-functional theory. <i>Physical Review A</i> , 2002, 66, .	1.0	3
1027	A theoretical study of the molecular structure and torsional potential of styrene. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2002, 35, 1509-1523.	0.6	43
1028	Absence of Dual Fluorescence in Cyano Isomers and Di-Cyano Derivatives Related to N,N-Dimethyl-4-Aminobenzonitril: A DFT/MRCI Study. <i>Zeitschrift Fur Physikalische Chemie</i> , 2002, 216, .	1.4	3
1029	Optimized structure of SiN _x Cy interfaces. <i>Semiconductor Science and Technology</i> , 2002, 17, 918-923.	1.0	2
1030	Exchange and correlation interplay in density functional theory under test: the relative stability of C ₃ H isomers. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2002, 35, 3689-3699.	0.6	7
1031	Magnetic-dipole, quadrupole-dipole and electron-vibration manifestations in chirality. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2002, 35, 4069-4076.	0.6	2
1032	Hybrid Density-Functional Calculations of the Reactions of a H ₂ Molecule on C, Si, and Ge(001) Surfaces. <i>Journal of Physical Chemistry B</i> , 2002, 106, 570-573.	1.2	18
1033	Transient Resonance Raman Spectroscopy and Density Functional Theory Investigation of Iso-Dibromoacetic Acid Photoproduct Produced From Ultraviolet Photolysis of Dibromoacetic Acid in the Solution Phase. <i>Bulletin of the Chemical Society of Japan</i> , 2002, 75, 943-948.	2.0	6
1034	The Hydration of Formic Acid. <i>Journal of Physical Chemistry A</i> , 2002, 106, 363-370.	1.1	101
1035	Evidence for HOOO Radicals in the Formation of Alkyl Hydrotrioxides (ROOOH) and Hydrogen Trioxide (HOOOH) in the Ozonation of C-H Bonds in Hydrocarbons ¹ . <i>Journal of the American Chemical Society</i> , 2002, 124, 404-409.	6.6	60
1036	Catalysis of H ₂ /D ₂ Scrambling and Other H/D Exchange Processes by [Fe]-Hydrogenase Model Complexes. <i>Inorganic Chemistry</i> , 2002, 41, 3917-3928.	1.9	249
1037	Computational and Experimental Studies of the Effect of Substituents on the Singlet-Triplet Energy Gap in Phenyl(carbomethoxy)carbene. <i>Journal of Organic Chemistry</i> , 2002, 67, 3079-3088.	1.7	39
1038	Theoretical Study on Chlorine and Hydrogen Shift in Cycloheptatriene and Cyclopentadiene Derivatives. <i>Journal of Organic Chemistry</i> , 2002, 67, 625-632.	1.7	42
1039	Absolute Configuration and Conformational Stability of (S)-(+)-3-(2-Methylbutyl)thiophene and 5918-5923.	1.1	19
1040	Mono- and Dinuclear Olefin Reactions at Aluminum. <i>Organometallics</i> , 2002, 21, 34-38.	1.1	18
1041	Hydrogen Adsorption on the Indium-Rich Indium Phosphide (001) Surface: A Novel Way to Produce Bridging In-H In Bonds. <i>Journal of the American Chemical Society</i> , 2002, 124, 15119-15124.	6.6	33
1042	Application of Time-Resolved Infrared Spectroscopy to Electronic Structure in Metal-to-Ligand Charge-Transfer Excited States. <i>Inorganic Chemistry</i> , 2002, 41, 6071-6079.	1.9	129
1043	Kinetically Favored Adsorbate Ordering: Hydrogen and Iodine on the Si(100)-2 × 1 Surface. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7286-7289.	1.2	20

#	ARTICLE	IF	CITATIONS
1044	Planar Transition Structures in the Epoxidation of Alkenes. A DFT Study on the Reaction of Peroxyformic Acid with Norbornene Derivatives. <i>Journal of Organic Chemistry</i> , 2002, 67, 8519-8527.	1.7	21
1045	Density Functional Theory Investigation of the Remarkable Reactivity of Geminal Dizinc Carbenoids (RZn) ₂ CHI (R = Et or I) as Cyclopropanation Reagents with Olefins Compared to Mono Zinc Carbenoids RZnCHI ₂ , EtCHI ₂ ZnR (R = Et or I). <i>Journal of the American Chemical Society</i> , 2002, 124, 12903-12914.	6.6	46
1046	A Computational Study of the Hydration of the OH Radical. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9104-9113.	1.1	59
1047	Computational Study of the Reactions of H Atoms with Chlorinated Alkanes. Isodesmic Reactions for Transition States. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11603-11615.	1.1	21
1048	Ab Initio Direct Dynamics Studies on the Reactions of H Atoms with CCl ₄ and CHCl ₃ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 12292-12298.	1.1	7
1049	Anion photoelectron spectroscopy of I ₂ ⁻ (CO) _n (n=1-8) clusters. <i>Journal of Chemical Physics</i> , 2002, 116, 6111-6117.	1.2	20
1050	Conformational Analysis of (S)-(+)-1-Bromo-2-methylbutane and the Influence of Bromine on Conformational Stability. <i>Journal of Physical Chemistry A</i> , 2002, 106, 12365-12369.	1.1	26
1051	Theoretical Studies of the Cross-Linking Mechanisms between Cytosine and Tyrosine. <i>Journal of the American Chemical Society</i> , 2002, 124, 2753-2761.	6.6	35
1052	An Experimental and Computational Evaluation of the Energetics of the Isomeric Methoxyphenylcarbenes Generated in Carbon Atom Reactions. <i>Journal of the American Chemical Society</i> , 2002, 124, 355-364.	6.6	21
1053	Kinetics of Reactions of Cl Atoms with Methane and Chlorinated Methanes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10532-10542.	1.1	68
1054	Modeling Copper(I) Complexes: A SIBFA Molecular Mechanics versus ab Initio Energetics and Geometrical Arrangements. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5660-5670.	1.1	35
1055	Nucleation dynamics in neon trimer photoionization: a time-dependent modelling. <i>Molecular Physics</i> , 2002, 100, 3699-3710.	0.8	4
1056	Theory Supplemented by Experiment. Electronic Effects on the Rotational Stability of the Amide Group in p-Substituted Acetanilides. <i>Journal of Organic Chemistry</i> , 2002, 67, 6210-6215.	1.7	27
1057	Theoretical Study of the Reaction XY ₄ = XY ₃ + Y, Where X = C, Si, Ge, Sn, Pb and Y = CH ₃ , C ₂ H ₅ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 7057-7061.	1.1	6
1058	Unimolecular Dissociation of Formyl Halides HXCO → CO + HX (X = F, Cl): An Ab Initio Direct Classical Trajectory Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11623-11629.	1.1	19
1059	Ab Initio CASSCF and DFT Investigations of (H ₂ O) ₂ ⁺ and (H ₂ S) ₂ ⁺ : Hemi-Bonded vs Proton-Transferred Structure. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11815-11821.	1.1	34
1060	Density Functional Theory Study of Alkali Metal-Noble Metal Diatomic Molecules. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11637-11643.	1.1	30
1061	Why Does Cp ₂ YH Catalyze the Polymerization of Ethene but Not of Propene?. <i>Organometallics</i> , 2002, 21, 1861-1869.	1.1	6

#	ARTICLE	IF	CITATIONS
1062	Competition between X \cdots H \cdots Y Intramolecular Hydrogen Bonds and X \cdots Y (X = O, S, and Y = Se, Te) Chalcogen \cdots Chalcogen Interactions. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4661-4668.	1.1	126
1063	Theoretical Investigation on Functionalization of Alkanes by a Rhodium Complex Catalyst. <i>Organometallics</i> , 2002, 21, 3703-3708.	1.1	54
1064	Kinetics of the Reaction Al + SF ₆ in the Temperature Range 499 \sim 813 K. <i>Journal of Physical Chemistry A</i> , 2002, 106, 307-311.	1.1	7
1065	Theoretical Calculation of Gas-Phase Sodium Binding Energies of Common MALDI Matrices. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6610-6617.	1.1	35
1066	Structures, Rotational Barriers, Thermochemical Properties, and Additivity Groups for 2-Propanol, 2-Chloro-2-propanol and the Corresponding Alkoxy and Hydroxyalkyl Radicals. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3947-3956.	1.1	25
1067	Density Functional Theory and ab Initio Direct Dynamics Studies on the Hydrogen Abstraction Reactions of Chlorine Atoms with CHCl ₃ -nFn (n = 0, 1, and 2) and CH ₂ Cl ₂ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 320-325.	1.1	20
1068	Computational Characterization of Sulfur \cdots Oxygen-Bonded Sulfuranyl Radicals Derived from Alkyl- and (Carboxyalkyl)thiopropionic Acids: Evidence for \dot{S}^* -Type Radicals. <i>Journal of Organic Chemistry</i> , 2002, 67, 1526-1535.	1.7	17
1069	Experimental Rate Measurements for NS + NO, O ₂ and NO ₂ , and Electronic Structure Calculations of the Reaction Paths for NS + NO ₂ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 8406-8410.	1.1	4
1070	Characteristics of Silver Ions Exchanged in ZSM-5-Type Zeolite, Aluminosilicate, and SiO ₂ Samples: A Comparison with the Properties of Copper Ions Exchanged in These Materials. <i>Journal of Physical Chemistry B</i> , 2002, 106, 8976-8987.	1.2	20
1071	Quantifying the Electronic Effect of Substituted Phosphine Ligands via Molecular Electrostatic Potential. <i>Inorganic Chemistry</i> , 2002, 41, 1573-1578.	1.9	157
1072	Addition of Organolithium Reagents to Corannulene and Conformational Preferences in 1-Alkyl-1,2-dihydrocorannulenes. <i>Journal of Organic Chemistry</i> , 2002, 67, 6487-6492.	1.7	20
1073	The Transition State for Intramolecular Atom Exchange between Hydride and Dihydrogen Ligands incis-[Fe(PR ₃) ₄ H(H ₂)] ₂ +Complexes. Trishydride or Trihydrogen?. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6189-6192.	1.1	12
1074	A Theoretical Study on the Two Reactions of Acetonitrile with Atomic Chlorine and Bromine. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8883-8890.	1.1	10
1075	Density Functional Theory Study of Atomic Nitrogen on the Si(100) $\sqrt{2 \times 2}$ Surface. <i>Journal of Physical Chemistry B</i> , 2002, 106, 2643-2648.	1.2	15
1076	Gas-Phase Basicity of 2,7-Dimethyl-[1,2,4]-Triazepine Thio Derivatives. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7383-7389.	1.1	18
1077	Coordination Chemistry of Silver Cations. <i>Journal of the American Chemical Society</i> , 2002, 124, 13613-13623.	6.6	90
1078	Vinylphosphirane \rightarrow Phospholene Rearrangements: A Pericyclic [1,3]-Sigmatropic Shifts or Not?. <i>Journal of the American Chemical Society</i> , 2002, 124, 13903-13910.	6.6	31
1079	Theoretical Study of Rhodium(III)-Catalyzed Hydrogenation of Carbon Dioxide into Formic Acid. Significant Differences in Reactivity among Rhodium(III), Rhodium(I), and Ruthenium(II) Complexes. <i>Journal of the American Chemical Society</i> , 2002, 124, 7588-7603.	6.6	103

#	ARTICLE	IF	CITATIONS
1080	Coordination Geometries of Zn(II) and Cd(II) in Phosphotriesterase: Influence of Water Molecules in the Active Site. <i>Journal of Physical Chemistry B</i> , 2002, 106, 9446-9453.	1.2	19
1081	Substituent Effects in the Interconversion of Phenylcarbene, Bicyclo[4.1.0]hepta-2,4,6-triene, and 1,2,4,6-Cycloheptatetraene. <i>Journal of Organic Chemistry</i> , 2002, 67, 2532-2540.	1.7	32
1082	N-Amination of Peptides: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1441-1449.	1.1	14
1083	Comparisons between Density Functional Theory and Conventional ab Initio Methods for 1,2-Elimination of HF from 1,1,1-Trifluoroethane: Test Case Study for HF Elimination from Fluoroalkanes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8471-8478.	1.1	25
1084	Structure, Bonding, and Spectra of Cyclic Dithia Radical Cations: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 8321-8328.	6.6	47
1085	A Self-Consistent Charge-Embedding Methodology for ab Initio Quantum Chemical Cluster Modeling of Ionic Solids and Surfaces: Application to the (001) Surface of Hematite (\pm -Fe ₂ O ₃). <i>Journal of Physical Chemistry B</i> , 2002, 106, 8136-8141.	1.2	31
1086	Comparison of Multireference Møller-Plesset Theory and Time-Dependent Methods for the Calculation of Vertical Excitation Energies of Molecules. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6844-6850.	1.1	123
1087	Determination of the Structures of Chiral Molecules Using Vibrational Circular Dichroism Spectroscopy. <i>ACS Symposium Series</i> , 2002, , 18-33.	0.5	22
1088	Density Functional Study of the Proline-Catalyzed Direct Aldol Reaction. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5155-5159.	1.1	188
1089	Proton-Coupled Electron Transfer in DNA-Acrylamide Complexes. <i>Journal of Physical Chemistry B</i> , 2002, 106, 8415-8421.	1.2	24
1090	Hydrogen-Bond Interactions in Organically-Modified Polysiloxane Networks Studied by 1D and 2D CRAMPS and Double-Quantum ¹ H MAS NMR. <i>Macromolecules</i> , 2002, 35, 10038-10047.	2.2	37
1091	Reactions between Glycolic Acid and Cu ⁺ in the Gas Phase. An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9359-9368.	1.1	19
1092	Atomic and Molecular Electron Affinities: Photoelectron Experiments and Theoretical Computations. <i>Chemical Reviews</i> , 2002, 102, 231-282.	23.0	1,152
1093	A Computational Study of the Isomerization of Prolyl Amides As Catalyzed by Intramolecular Hydrogen Bonding. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11168-11172.	1.1	23
1094	Combined Spectroelectrochemical and Theoretical Study of a Vinylene-Bridged Sexithiophene Cooligomer: Analysis of the π -Electron Delocalization and of the Electronic Defects Generated upon Doping. <i>Journal of Physical Chemistry B</i> , 2002, 106, 3872-3881.	1.2	63
1095	Possible Strategies toward the Elusive Tetraaminodisilene. <i>Journal of the American Chemical Society</i> , 2002, 124, 3457-3460.	6.6	15
1096	Mechanism of the Six-Electron Reduction of Nitrite to Ammonia by Cytochrome c Nitrite Reductase. <i>Journal of the American Chemical Society</i> , 2002, 124, 11737-11745.	6.6	292
1097	In Vitro Biotransformation of (R)- and (S)-Thalidomide: Application of Circular Dichroism Spectroscopy to the Stereochemical Characterization of the Hydroxylated Metabolites. <i>Analytical Chemistry</i> , 2002, 74, 3726-3735.	3.2	50

#	ARTICLE	IF	CITATIONS
1098	A critical note on density functional theory studies on rare-gas dimers. <i>Journal of Chemical Physics</i> , 2002, 116, 9620-9623.	1.2	221
1099	Selectivity of Metallocene-Catalyzed Olefin Polymerization: A Combined Experimental and Quantum Mechanical Study. 1. Nonchiral Bis(cyclopentadienyl) Systems. <i>Macromolecules</i> , 2002, 35, 2835-2844.	2.2	36
1100	Tuning the Electronic Structure of Octahedral Iron Complexes [FeL(X)] (L = Alkyl-4,7-bis(4-tert-butyl-2-mercaptobenzyl)-1,4,7-triazacyclononane, X = Cl, CH ₃ O, CN, NO). The S = 1/2 ↔ S = 3/2 Spin Equilibrium of [FeLPr(NO)]. <i>Inorganic Chemistry</i> , 2002, 41, 3444-3456.	1.9	102
1101	Bonding in the oxo ferrous iron species: A complete active-space self-consistent-field theory verification of the molecular-oxygen-like pattern. <i>Journal of Chemical Physics</i> , 2002, 117, 7153-7161.	1.2	18
1102	Calculation of exchange integrals and electronic structure for manganese ferrite. <i>Physical Review B</i> , 2002, 66, .	1.1	25
1103	A Comparative Theoretical Study on DMABN: Significance of Excited State Optimized Geometries and Direct Comparison of Methodologies. <i>Journal of Physical Chemistry A</i> , 2002, 106, 804-815.	1.1	65
1104	Hybrid Density-Functional Theory and the Insulating Gap of UO ₂ . <i>Physical Review Letters</i> , 2002, 89, 266402.	2.9	329
1105	Electron Affinity of the Guanine-Cytosine Base Pair and Structural Perturbations upon Anion Formation. <i>Journal of the American Chemical Society</i> , 2002, 124, 10163-10170.	6.6	125
1106	Nitro derivatives of pyrrole, furan and 1H-tetrazole: ring or nitro bases?. <i>New Journal of Chemistry</i> , 2002, 26, 1567-1574.	1.4	14
1107	Density function studies of peptides. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 1490-1499.	1.3	19
1108	Synthesized rare-earth doped oxide glasses for nonlinear optics. <i>Journal of Applied Physics</i> , 2002, 92, 2260-2268.	1.1	38
1109	Charge Model 3: A Class IV Charge Model Based on Hybrid Density Functional Theory with Variable Exchange. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10707-10717.	1.1	48
1110	DENSITY FUNCTIONAL THEORY: In Pursuit of the. <i>Science</i> , 2002, 298, 759-760.	6.0	129
1111	Theoretical study of the hydrogen abstraction by chlorine atoms for CH ₂ BrCl and CHBrCl ₂ . <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 46-50.	1.3	4
1112	Validation study of meta-GGA functionals and of a model exchange-correlation potential in density functional calculations of EPR parameters. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5467-5474.	1.3	67
1113	Structures, thermochemical properties (enthalpy, entropy and heat capacity), rotation barriers, and peroxide bond energies of vinyl, allyl, ethynyl and phenyl hydroperoxides Electronic supplementary information (ESI) available. Structures, geometry parameters, thermochemical properties, rotation barriers and peroxide bond energies of vinyl, allyl, ethynyl and phenyl hydroperoxides. See http://www.rsc.org/suppdata/cp/b1/b111303h Presented at the Bunsen Discussion on Formation and Degradation of Hydrocarbons I. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 3691-3703.	1.3	60
1114	Infrared Matrix Isolation Studies and Ab Initio Calculations of Formhydroxamic Acid. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3714-3721.	1.1	26
1115	New Sorbents for Desulfurization by π-Complexation: Thiophene/Benzene Adsorption. <i>Industrial & Engineering Chemistry Research</i> , 2002, 41, 2487-2496.	1.8	226

#	ARTICLE	IF	CITATIONS
1116	An ab Initio Quantum Mechanical Study of Hydrogen-Bonded Complexes of Biological Interest. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7820-7827.	1.1	49
1117	Relative Acidities of Ortho-Substituted Phenols, as Models for Modified Tyrosines in Proteins. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8757-8761.	1.1	41
1118	Analysis of the effect of changing the α_0 parameter of the Becke3-LYP hybrid functional on the transition state geometries and energy barriers in a series of prototypical reactions. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 722-731.	1.3	51
1119	Cyclic Vinylp-Tolyl Sulfilimines as Chiral Dienophiles: A Theoretical Study on the Stereoselectivity, Lewis Acid Catalysis, and Solvent Effects in Their Diels-Alder Reactions. <i>Journal of Organic Chemistry</i> , 2002, 67, 2926-2933.	1.7	10
1120	Gas-Phase Chemistry of Ethyl and Vinyl Amines, Phosphines, and Arsines: A DFT Study of the Structure and Stability of Their Cu^+ Complexes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9306-9312.	1.1	10
1121	Density Functional Theory Investigation of the Reaction of Isodiiodomethane with Acetylene: Potential Utility of Isodiiodomethane for Cyclopropanation Reactions. <i>Journal of Organic Chemistry</i> , 2002, 67, 4619-4622.	1.7	2
1122	Nonstatistical Translational Energy Distribution of H_2 Elimination Products from $\text{Co}^+(3\text{F}_4) + \text{Propane}$. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5563-5576.	1.1	32
1123	Quinonoid Oligothiophenes as Electron-Donor and Electron-Acceptor Materials. A Spectroelectrochemical and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 12380-12388.	6.6	109
1124	DFT study of the rate constants of the reactions $\text{CH}_3\text{I} + \text{F}_3\text{A}^{\sim} \rightarrow \text{CH}_3\text{Cl} + \text{F}_3\text{A}^{\sim} + \text{HF}$ ($\text{A} = \text{C}, \text{Si}$). <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 4386-4391.	1.3	5
1125	Density functional theory investigation of the reactions of CH_2BrI , CH_2IBr , CH_2ClI , and CH_2ICl isopolyhalomethanes with ethylene. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5059-5065.	1.3	6
1126	An ab initio direct classical trajectory study of s-tetrazine photodissociation. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 2554-2559.	1.3	8
1127	Ferroelectric liquid crystal induced by a bridged biphenyl dopant with helical topography. <i>Journal of Materials Chemistry</i> , 2002, 12, 586-592.	6.7	16
1128	Coupling of solvent and solute dynamics in molecular dynamics simulations of aqueous urea solutions with different intramolecular potentials. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 86-95.	1.3	49
1129	Tools of the trade in modeling inorganic reactions. From balls and sticks to HOMO's and LUMO's. Based on the presentation given at Dalton Discussion No. 4, 10 th January 2002, Kloster Banz, Germany. <i>Dalton Transactions RSC</i> , 2002, , 642-652.	2.3	37
1130	Crystal chemistry of tetraradial species. Part 10. Tilting at windmills: conformations of the tetraphenyl species ZPh_4 , $\Delta \pm 1$ ($Z = \text{B}, \text{C}, \text{N}$). <i>Canadian Journal of Chemistry</i> , 2002, 80, 1351-1366.	0.6	16
1131	Understanding the unusual g-values and the spin density distribution of hydrogen atoms trapped in silasesquioxanes. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5458-5466.	1.3	14
1132	Instability of a system and its estimation in terms of the hybrid density functional theory method: a magnetic effective density functional (MEDF) approach. <i>Molecular Physics</i> , 2002, 100, 1829-1838.	0.8	26
1133	Ring structure of the NO dimer radical cation: A possible new assignment of the mysterious IR absorption at 1424 cm^{-1} . <i>Journal of Chemical Physics</i> , 2002, 117, 9727-9732.	1.2	8

#	ARTICLE	IF	CITATIONS
1134	Isotope effects in the electron impact ionization of H ₂ /D ₂ , H ₂ O/D ₂ O, and C ₆ H ₆ /C ₆ D ₆ near threshold. <i>Journal of Chemical Physics</i> , 2002, 116, 2456-2463.	1.2	38
1135	Ab initio investigation of the gas phase reaction SO ₂ + H ₂ O → SO ₂ OH radical. <i>Molecular Physics</i> , 2002, 100, 1847-1853.	0.8	6
1136	Water dissolution in albite melts. <i>Geochimica Et Cosmochimica Acta</i> , 2002, 66, 4149-4163.	1.6	19
1137	Outer-sphere electron transfer kinetics of metal ion oxidation by molecular oxygen. <i>Geochimica Et Cosmochimica Acta</i> , 2002, 66, 4223-4233.	1.6	72
1138	Molecular Dynamics Study of <i>Desulfovibrio africanus</i> Cytochrome c3 in Oxidized and Reduced Forms. <i>Biophysical Journal</i> , 2002, 83, 3049-3065.	0.2	12
1139	Hybrid Density Functional Theory Studies on the Magnetic Interactions and the Weak Covalent Bonding for the Phenalenyl Radical Dimeric Pair. <i>Journal of the American Chemical Society</i> , 2002, 124, 11122-11130.	6.6	118
1140	Electronic Structure and Reactivity of Low-Spin Fe(III)-Hydroperoxo Complexes: Comparison to Activated Bleomycin. <i>Journal of the American Chemical Society</i> , 2002, 124, 10810-10822.	6.6	121
1141	Computational Studies on Biphenyl Derivatives. Analysis of the Conformational Mobility, Molecular Electrostatic Potential, and Dipole Moment of Chlorinated Biphenyl: Searching for the Rationalization of the Selective Toxicity of Polychlorinated Biphenyls (PCBs). <i>Chemical Research in Toxicology</i> , 2002, 15, 1514-1526.	1.7	69
1142	Catalytic Mechanism of Matrix Metalloproteinases: A Two-Layered ONIOM Study. <i>Inorganic Chemistry</i> , 2002, 41, 5659-5666.	1.9	100
1143	A Molecular Electrostatic Potential Bond Critical Point Model for Atomic and Group Electronegativities. <i>Journal of the American Chemical Society</i> , 2002, 124, 1790-1797.	6.6	73
1144	Implicit and Explicit Coverage of Multi-reference Effects by Density Functional Theory. <i>International Journal of Molecular Sciences</i> , 2002, 3, 604-638.	1.8	111
1145	A computational study of conformers of 1,3-dioxane (1,3-dioxacyclohexane). <i>Computational and Theoretical Chemistry</i> , 2002, 577, 43-54.	1.5	37
1146	Mechanism analysis of catalytic hydrogenation of 3-anilinomethylidene-6-alkyl-5,6,2H-dihydropyran-2,4-diones. <i>Computational and Theoretical Chemistry</i> , 2002, 578, 71-78.	1.5	2
1147	How accurately can we calculate molecular CH and CC re distances by DFT methods? Dependence on basis sets and functionals, estimations of experimentally inaccessible re distances and distance-dependent scaling factors for approximations of triple-zeta quality. <i>Computational and Theoretical Chemistry</i> , 2002, 578, 229-247.	1.5	16
1148	Experimental and calculated molecular structures and high symmetry conformations of [Sb ₂ F ₁₁] ⁺ (D _{4h}) and 1,4-C ₄ H ₄ N ₂ ·2SbF ₅ (D _{2h}). <i>Solid State Sciences</i> , 2002, 4, 1457-1463.	1.5	18
1150	Aromatische Borane mit planar-tetrakoordinierten Boratomen und sehr kurzen B-B-Abständen. <i>Angewandte Chemie</i> , 2002, 114, 1597-1599.	1.6	31
1151	Synthesis of 1-Azaspiro[2.4]hepta-1,4,6-trienes and Azaspiroconjugation Studied by Photoelectron Spectroscopy. <i>Chemistry - A European Journal</i> , 2002, 8, 5089-5093.	1.7	11
1152	Sigmatropic Shiftamers: Fluxionality in Broken Ladderane Polymers. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1033-1036.	7.2	35

#	ARTICLE	IF	CITATIONS
1153	Aromatic Boranes with Planar-Tetracoordinate Boron Atoms and Very Short Bâ~B Distances. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1526-1529.	7.2	53
1154	Synthesis, X-ray Structures, NMR Studies and Density Functional Calculations of (Î-2-Fumarodinitrile)palladium(0) Complexes Containing Dihydro(phosphanylphenyl)oxazole Ligands. <i>European Journal of Inorganic Chemistry</i> , 2002, 2002, 1511-1517.	1.0	11
1155	The Synthesis and Configurational Stability of Enantioenriched Î±-Thioallyllithium Compounds and the Stereochemical Course of Their Electrophilic Substitution. <i>European Journal of Organic Chemistry</i> , 2002, 2002, 2970-2988.	1.2	21
1156	Photoelectron Spectra, Electronic Structures, and Conformational Properties of Substituted 2-Styrylpyrroles. <i>European Journal of Organic Chemistry</i> , 2002, 2002, 551-556.	1.2	7
1157	Development of a Working Model of the Active Site in Bovine Lens Leucine Aminopeptidase: A Density Functional Investigation. <i>ChemBioChem</i> , 2002, 3, 101-104.	1.3	19
1158	Photoelectron Spectra and Electronic Structure of Some Diastereomeric Quinuclidine Derivatives. <i>ChemPhysChem</i> , 2002, 3, 957-962.	1.0	3
1159	New adsorbents for purification: Selective removal of aromatics. <i>AIChE Journal</i> , 2002, 48, 1457-1468.	1.8	29
1160	Interaction of Cu ⁺ and Cu ²⁺ ions with Î-glycyl-L-alanine. A density functional study. <i>Journal of Mass Spectrometry</i> , 2002, 37, 786-791.	0.7	38
1161	Substituent effects on ¹ H and ¹³ C NMR chemical shifts in Î-monosubstituted ethyl acetates: principal component analysis and ¹ H chemical shift calculations. <i>Magnetic Resonance in Chemistry</i> , 2002, 40, 449-454.	1.1	13
1162	Absolute configuration and conformational analysis of a degradation product of inhalation anesthetic Sevoflurane: A vibrational circular dichroism study. <i>Chirality</i> , 2002, 14, 618-624.	1.3	13
1163	A Correlation for Establishing Solvolysis Rates of Aqueous Al(III) Complexes: A Possible Strategy for Colloids and Nanoparticles. <i>Journal of Colloid and Interface Science</i> , 2002, 251, 1-9.	5.0	5
1164	Planarity of acetamides, thioacetamides, and selenoacetamides: Crystal structure of N,N-dimethylselenoacetamide. <i>Heteroatom Chemistry</i> , 2002, 13, 380-386.	0.4	7
1165	Studies on 4,7-di-substitution effects of one ligand in [Ru(Phen) ₃] ₂ with DFT method. <i>Journal of Computational Chemistry</i> , 2002, 23, 436-443.	1.5	21
1166	Calculation of electronic g-tensors for transition metal complexes using hybrid density functionals and atomic meanfield spin-orbit operators. <i>Journal of Computational Chemistry</i> , 2002, 23, 794-803.	1.5	182
1167	Ab initio conformational studies on diols and binary diol-water systems using DFT methods. Intramolecular hydrogen bonding and 1:1 complex formation with water. <i>Journal of Computational Chemistry</i> , 2002, 23, 585-599.	1.5	104
1168	Spin-orbit coupling of DFT/MRCI wavefunctions: Method, test calculations, and application to thiophene. <i>Journal of Computational Chemistry</i> , 2002, 23, 824-833.	1.5	145
1169	Binding of D- and L-captopril inhibitors to metallo-Î²-lactamase studied by polarizable molecular mechanics and quantum mechanics. <i>Journal of Computational Chemistry</i> , 2002, 23, 1281-1296.	1.5	57
1170	DFT and Ab initio direct dynamics studies on the hydrogen abstraction reactions of chlorine atoms with CH ₄ ?nFn (n = 1-3). <i>Journal of Computational Chemistry</i> , 2002, 23, 1456-1465.	1.5	4

#	ARTICLE	IF	CITATIONS
1171	Molecules for materials: Germanium hydride neutrals and anions. Molecular structures, electron affinities, and thermochemistry of GeH _n /GeH _n ⁻ (n = 0-4) and Ge ₂ H _n /Ge ₂ H _n ⁻ (n = 0-6). Journal of Computational Chemistry, 2002, 23, 1642-1655.	1.5	41
1172	Are allylic hydrogens in catechins more abstractable than catecholic hydrogens?. JAOCS, Journal of the American Oil Chemists' Society, 2002, 79, 943-944.	0.8	14
1173	Peroxy adduct radicals formed in the iron/oxygen reconstitution reaction of mutant ribonucleotide reductase R2 proteins from Escherichia coli. Journal of Biological Inorganic Chemistry, 2002, 7, 74-82.	1.1	6
1174	Density functional models of the mechanism for decarboxylation in orotidine decarboxylase. Journal of Molecular Modeling, 2002, 8, 119-130.	0.8	15
1175	The 1.76 Å... Resolution Crystal Structure of Glycogen Phosphorylase b Complexed with Glucose, and CP320626, a Potential Antidiabetic Drug. Bioorganic and Medicinal Chemistry, 2002, 10, 1313-1319.	1.4	32
1176	Density functional studies of catalytic alkane dehydrogenation by an iridium pincer complex with and without a hydrogen acceptor. Journal of Molecular Catalysis A, 2002, 189, 111-118.	4.8	15
1177	Dissociation behavior of ionized valeramide. International Journal of Mass Spectrometry, 2002, 214, 129-154.	0.7	16
1178	Hydrogen-shift isomers of ionic and neutral hydroxypyridines: a combined experimental and computational investigation. International Journal of Mass Spectrometry, 2002, 217, 1-22.	0.7	25
1179	Distonic isomers of ionized benzaldehyde. International Journal of Mass Spectrometry, 2002, 217, 65-73.	0.7	9
1180	Small carbon clusters (C _n O, C _n ⁺ , C _n ⁻) from acyclic and cyclic precursors. International Journal of Mass Spectrometry, 2002, 217, 81-96.	0.7	26
1181	Modelling ionic nucleation in small neon clusters. International Journal of Mass Spectrometry, 2002, 220, 193-209.	0.7	12
1182	Structures, thermochemistry, and infrared spectra of chloride ion-fluorinated acetone complexes and neutral fluorinated acetones in the gas phase: experiment and theory. International Journal of Mass Spectrometry, 2002, 219, 593-613.	0.7	11
1183	Generation and characterization of ionic and neutral P(OH) ₂ ⁺ in the gas phase by tandem mass spectrometry and computational chemistry. Journal of the American Society for Mass Spectrometry, 2002, 13, 250-264.	1.2	11
1184	On the reaction of mutagenic aflatoxin B1 oxide and benz[a]pyrene diol oxide with guanine residue in DNA double helix. Computational and Theoretical Chemistry, 2002, 581, 157-166.	1.5	6
1185	Direct ab initio dynamics and theoretical rate constants studies for hydrogen-abstraction reactions of chlorine atoms with dibromomethane and tribromomethane. Computational and Theoretical Chemistry, 2002, 582, 53-60.	1.5	2
1186	Tetrasulfur tetranitride and its selenium analogs: ab initio and DFT calculations. Computational and Theoretical Chemistry, 2002, 582, 85-90.	1.5	9
1187	Theoretical studies on the electronic structures and related properties of [Ru(L) ₃] ²⁺ (L=bpy, bpm,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.5	27
1188	Protonated cyclopropane as an intermediate in cation-olefin cyclizations. Ab initio and density functional theory investigations. Computational and Theoretical Chemistry, 2002, 589-590, 7-26.	1.5	3

#	ARTICLE	IF	CITATIONS
1189	Reliability of ab initio (HF, post HF and DFT) methods and basis set dependencies for accurate prediction of equilibrium r e distances of CO bond lengths. Computational and Theoretical Chemistry, 2002, 585, 35-47.	1.5	11
1190	The axial N -base has minor influence on Coâ€C bond cleavage in cobalamins. Computational and Theoretical Chemistry, 2002, 585, 239-255.	1.5	64
1191	Existence of hydrogen bonding between the hydrogen sulfide and hydroperoxy radical: H2SÂHO2. Computational and Theoretical Chemistry, 2002, 586, 149-157.	1.5	10
1192	A theoretical study of electrocyclizations of dienylketenes to cyclohexadienones: an AM1 study. Computational and Theoretical Chemistry, 2002, 589-590, 111-123.	1.5	6
1193	Theoretical molecular structures for partially bonded complexes of trimethylamine with SO2 and SO3: ab initio and density functional theory calculations. Computational and Theoretical Chemistry, 2002, 594, 147-156.	1.5	6
1194	Computational probes into the conceptual basis of silver ion chromatography: I. Silver(I) ion complexes of unsaturated fatty acids and esters. Computational and Theoretical Chemistry, 2002, 589-590, 239-249.	1.5	21
1195	Further studies on the rotational barriers of Carbamates. An NMR and DFT analysis of the solvent effect for Cyclohexyl N,N-dimethylcarbamate. Computational and Theoretical Chemistry, 2002, 594, 199-206.	1.5	24
1196	The use of ab initio and DFT calculations in the interpretation of ultraviolet photoelectron spectra: the rotational isomerism of anisole and thioanisole as a case study. Computational and Theoretical Chemistry, 2002, 618, 155-164.	1.5	23
1197	Evaluation of the effectiveness of AM1 geometry used in calculating Oâ€H bond dissociation enthalpy. Computational and Theoretical Chemistry, 2002, 618, 181-189.	1.5	8
1198	Formation of bis (chloromethyl) ether in the vapor phase: a computational investigation. Computational and Theoretical Chemistry, 2002, 619, 207-228.	1.5	5
1199	Direct ab initio dynamics studies on hydrogen-abstraction reactions of 1,1,1-trifluoroethane with hydroxyl radical. Chemical Physics, 2002, 282, 1-8.	0.9	3
1200	Adiabatic connection method for X??+?RX nucleophilic substitution reactions (X=?F, Cl). Journal of Physical Organic Chemistry, 2002, 15, 712-720.	0.9	34
1201	Brueckner orbitals and density-functional theory. International Journal of Quantum Chemistry, 2002, 90, 294-308.	1.0	48
1202	Structure and spin-state energetics of an iron porphyrin model: An assessment of theoretical methods. International Journal of Quantum Chemistry, 2002, 87, 158-166.	1.0	74
1203	An embedded QM/MM study for different SiO2/Al2O3ratios of the HZSM-5 zeolite and for their interaction with n-heptane. International Journal of Quantum Chemistry, 2002, 88, 750-766.	1.0	12
1204	Density functional complete study of hydrogen bonding between the water molecule and the hydroxyl radical (H2O Â HO). International Journal of Quantum Chemistry, 2002, 89, 550-558.	1.0	52
1205	Complexes of C60 fullerene with simple donor molecules: Theoretical study. International Journal of Quantum Chemistry, 2002, 89, 477-483.	1.0	24
1206	HF-CC model for atoms and molecules. International Journal of Quantum Chemistry, 2002, 90, 1295-1308.	1.0	0

#	ARTICLE	IF	CITATIONS
1207	Theoretical studies on the hydrolysis of phosphate diesters in the gas phase, solution, and RNase A. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 10-26.	1.0	41
1208	EPR observation of cathodically-generated radical anions of colchicidic and isocolchicidic, and a comparison with the radical anions of troponoids. A general rationalization of the spin-density distribution in these systems. <i>Tetrahedron</i> , 2002, 58, 9553-9558.	1.0	4
1209	Conformational stability and vibrational spectrum of glyoxilic acid oxime predicted from ab initio study. <i>Journal of Molecular Structure</i> , 2002, 604, 211-220.	1.8	9
1210	Structure and properties of N-methyl-N-(4-pyridyl)-nitramine and 1,4-dihydro-1-methyl-4-nitriminopyridine. <i>Journal of Molecular Structure</i> , 2002, 605, 157-169.	1.8	7
1211	¹ H and ¹³ C NMR spectroscopy of 9-acridinones. <i>Journal of Molecular Structure</i> , 2002, 612, 29-38.	1.8	9
1212	Isolation of a stable Cr(V) intermediate in the oxidation of aryl-substituted alkenes by chromylchloride. <i>Journal of Organometallic Chemistry</i> , 2002, 641, 121-125.	0.8	4
1213	Predictions of nitrogen isotropic hyperfine coupling constants in the nitroxide radicals with the aid of DF/HF calculations. <i>Journal of Solid State Chemistry</i> , 2002, 169, 75-80.	1.4	14
1214	On the evaluation of thermal corrections to gas phase ab initio relative energies: implications to the conformational analysis study of cyclooctane. <i>Chemical Physics</i> , 2002, 280, 31-42.	0.9	35
1215	DFT calculation on the energy thresholds of DNA damages under irradiation conditions. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2002, 300, 421-426.	0.9	6
1216	Studies on effects of di-F-substitution sites in main ligand of [Ru(bpy) ₂ (dpq)] ²⁺ with DFT method. <i>Inorganica Chimica Acta</i> , 2002, 335, 100-106.	1.2	12
1217	Prediction and interpretation of the ⁵⁷ Fe isomer shift in Mössbauer spectra by density functional theory. <i>Inorganica Chimica Acta</i> , 2002, 337, 181-192.	1.2	547
1218	A comparison of dioxygen bond-cleavage in ribonucleotide reductase (RNR) and methane monooxygenase (MMO). <i>Chemical Physics Letters</i> , 2002, 351, 311-318.	1.2	39
1219	Impact of conformation on the dipole moment of bis-triarylamine derivatives. <i>Chemical Physics Letters</i> , 2002, 354, 283-290.	1.2	33
1220	Collisionally induced loss of NO ₂ radical from protonated nitroimidazoles and nitropyrazoles. <i>Chemical Physics Letters</i> , 2002, 356, 259-266.	1.2	8
1221	Ionization potentials of small tin clusters: first principles calculations. <i>Chemical Physics Letters</i> , 2002, 356, 36-42.	1.2	17
1222	The nature of the Au-Rg bond in the [AuRg ₄] ²⁺ (Rg=Ar, Kr and Xe) molecules. <i>Chemical Physics Letters</i> , 2002, 356, 483-489.	1.2	30
1223	Effective exchange integrals and chemical indices for a phenalenyl radical dimeric pair. <i>Chemical Physics Letters</i> , 2002, 358, 17-23.	1.2	31
1224	Generation and characterization of ionic and neutral silicon dihydroxide Si(OH) ₂ ⁺⁰ and silanoic acid HSi(O)OH ⁺⁰ in the gas phase by tandem mass spectrometry and computational chemistry. <i>Chemical Physics Letters</i> , 2002, 360, 294-303.	1.2	11

#	ARTICLE	IF	CITATIONS
1225	Kinetics and thermodynamics of the Al+trimethylaluminum reaction. <i>Chemical Physics Letters</i> , 2002, 360, 313-319.	1.2	6
1226	Density functional theory direct dynamics study on the hydrogen abstraction reaction of CF ₃ CHFCF ₃ +OH ⁺ CF ₃ CF ₃ +H ₂ O. <i>Chemical Physics Letters</i> , 2002, 362, 39-46.	1.2	8
1227	Density functional theory study of CS ₂ /Cl adducts and their isomerization reactions. <i>Chemical Physics Letters</i> , 2002, 362, 205-209.	1.2	7
1228	Existence of hydroperoxy and hydrogen peroxide radical complex (HO ₂ ·H ₂ O ₂). <i>Chemical Physics Letters</i> , 2002, 366, 260-266.	1.2	19
1229	Molecular orbital study on the ground and excited states of methyl substituted tris(8-hydroxyquinoline) aluminum(III). <i>Chemical Physics Letters</i> , 2002, 366, 9-16.	1.2	44
1230	Density functional theory study of the canthaxanthin and other carotenoid radical cations. <i>Chemical Physics Letters</i> , 2002, 366, 73-81.	1.2	26
1231	Theoretical study of the reaction of Fe ⁺ with CS ₂ in gas phase. <i>Chemical Physics Letters</i> , 2002, 366, 253-259.	1.2	26
1232	Geometric and Electronic Structure of WSiN(N = 1-6, 12) Clusters. <i>Structural Chemistry</i> , 2002, 13, 173-191.	1.0	65
1233	Title is missing!. <i>Russian Journal of Electrochemistry</i> , 2002, 38, 111-122.	0.3	16
1234	Structural Study of Ni(dpm) ₂ in Solution by X-Ray Absorption Spectroscopy. <i>Journal of Structural Chemistry</i> , 2002, 43, 257-265.	0.3	0
1235	Title is missing!. <i>Journal of Structural Chemistry</i> , 2002, 43, 519-522.	0.3	0
1236	Title is missing!. <i>Russian Journal of Electrochemistry</i> , 2002, 38, 1339-1345.	0.3	4
1237	Atomistic mechanism of the initial oxidation of the clean Si(100)-(2×1) surface by O ₂ and SiO ₂ decomposition. <i>Journal of Chemical Physics</i> , 2002, 116, 5774-5780.	1.2	39
1238	Theoretical Elucidation on the Antioxidant Mechanism of Curcumin: A DFT Study. <i>Organic Letters</i> , 2002, 4, 2909-2911.	2.4	159
1239	Adiabatic time-dependent density functional methods for excited state properties. <i>Journal of Chemical Physics</i> , 2002, 117, 7433-7447.	1.2	1,992
1240	Unified Mechanistic Concept of Electrophilic Aromatic Nitration: Convergence of Computational Results and Experimental Data. <i>Journal of the American Chemical Society</i> , 2003, 125, 4836-4849.	6.6	142
1241	Electronic Structure and Reactivity of High-Spin Iron ^{IV} -Alkyl- and ^{IV} -Pterinperoxo Complexes. <i>Inorganic Chemistry</i> , 2003, 42, 469-481.	1.9	34
1242	Melting, volatilisation and crystal lattice enthalpies of acridin-9(10H)-ones. <i>Journal of Thermal Analysis and Calorimetry</i> , 2003, 74, 443-450.	2.0	15

#	ARTICLE	IF	CITATIONS
1243	Computational Study of Endohedral IrSi9+Isomers. <i>Structural Chemistry</i> , 2003, 14, 487-496.	1.0	3
1244	Computational studies of ice defects. <i>Canadian Journal of Physics</i> , 2003, 81, 325-332.	0.4	1
1245	The catalytic cycle of tyrosinase: peroxide attack on the phenolate ring followed by O-O bond cleavage. <i>Journal of Biological Inorganic Chemistry</i> , 2003, 8, 567-576.	1.1	80
1246	A comparison of the thermodynamics of O-O bond cleavage for dicopper complexes in enzymes and synthetic systems. <i>Journal of Biological Inorganic Chemistry</i> , 2003, 8, 577-585.	1.1	46
1247	Molecular dynamics in ferroelectric 4-aminopyridinium tetrachloroantimonate(III), [4-NH ₂ C ₅ H ₄ NH][SbCl ₄]. <i>Solid State Nuclear Magnetic Resonance</i> , 2003, 24, 209-217.	1.5	19
1248	A theoretical investigation on DPPH radical-Scavenging mechanism of edaravone. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2003, 13, 3789-3792.	1.0	63
1249	Theoretical study of low-lying electronic states of BP molecule. <i>Chemical Physics Letters</i> , 2003, 381, 720-724.	1.2	8
1250	Modeling water exchange on monomeric and dimeric Mn centers. <i>Theoretical Chemistry Accounts</i> , 2003, 110, 130-143.	0.5	35
1251	Catalysis by methyl-coenzyme M reductase: a theoretical study for heterodisulfide product formation. <i>Journal of Biological Inorganic Chemistry</i> , 2003, 8, 653-662.	1.1	70
1252	A computer-aided quantum chemical study of the N 15 π^* cluster. <i>Journal of Molecular Modeling</i> , 2003, 9, 99-107.	0.8	8
1253	Nonradical mechanism of (bi)sulfite reaction with DEPMPO: cautionary note for SO ₃ \cdot^- radical spin trapping. <i>Free Radical Biology and Medicine</i> , 2003, 34, 196-206.	1.3	17
1254	On the thermal decomposition pathway of coordination compounds: synthesis, crystal structures and properties of new polymorphic CuI(2-ethylpyrazine) coordination compounds. <i>Solid State Sciences</i> , 2003, 5, 1343-1357.	1.5	28
1255	Gas-Phase Chemistry of Ethynylamine, -Phosphine and -Arsine. Structure and Stability of their Cu ⁺ and Ni ⁺ Complexes. <i>ChemPhysChem</i> , 2003, 4, 72-78.	1.0	5
1256	Helicoid Shiftamers for the Transport of π -Clumps and Charges. <i>Helvetica Chimica Acta</i> , 2003, 86, 3525-3532.	1.0	9
1257	Performance assessment of density-functional methods for study of charge-transfer complexes. <i>Journal of Computational Chemistry</i> , 2003, 24, 623-631.	1.5	79
1258	Hydrogen bonding in diols and binary diol-water systems investigated using DFT methods. II. Calculated infrared OH-stretch frequencies, force constants, and NMR chemical shifts correlate with hydrogen bond geometry and electron density topology. A reevaluation of geometrical criteria for hydrogen bonding. <i>Journal of Computational Chemistry</i> , 2003, 24, 1120-1131.	1.5	79
1259	A comparison of the mechanism for the reductive half-reaction between pea seedling and other copper amine oxidases (CAOs). <i>Journal of Computational Chemistry</i> , 2003, 24, 1599-1609.	1.5	4
1260	NIR Dyes Based on [M(R ₂ timdt) ₂] Metal-Dithiolenes: Additivity of M, R, and R ² Contributions To Tune the NIR Absorption (M = Ni, Pd, Pt; R, R ² timdt = Monoreduced Form of Disubstituted) Tj ETQq1 1 0.784314 rgBT /Overlock 10 1650 57	1.0	1

#	ARTICLE	IF	CITATIONS
1261	Synthesis, Kinetic Study and Molecular Orbital Investigation of Cadmium(II), Mercury(II) and Lead(II) Complexes with the Mixed Pendant-Arm Macrocyclic Ligand 1,7-Bis(carboxymethyl)-4,10-bis(1-methylimidazol-2-ylmethyl)-1,4,7,10-tetraazacyclododecane. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 3185-3192.	1.0	4
1262	Bent and Linear Forms of the (1/4-Oxo)bis[trichloroferrate(III)] Dianion: An Intermolecular Effect? Structural, Electronic and Magnetic Properties. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 4187-4194.	1.0	10
1263	2,3-Bis(diarylphosphanyl)-1,4-diazadienes: P,P Coordination of PdII, PtII and a Nickelacyclopentanone with Subsequent Formation of Quinoxalines by a Ring-Closure Reaction at the Periphery. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 4321-4331.	1.0	11
1264	A Facile Synthesis of a Push-Pull Mixed-Ligand Pd-Dithiolene Complex Containing the Et2timdt Ligand (Et2timdt = Monoreduced Diethylimidazolidine-2,4,5-trithione). <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 1291-1295.	1.0	9
1265	Structures of Carbonato and Bicarbonato Complexes of Bis(1,10-phenanthroline)Zinc(II): Experiment and Theory. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 1562-1569.	1.0	15
1266	Raman spectroscopy, surface-enhanced Raman spectroscopy and density functional theory studies of 2-formylfuran. <i>Journal of Raman Spectroscopy</i> , 2003, 34, 705-710.	1.2	6
1267	Radical Cation, Dimer Radical Cation and Neutral Radical of 2,3-Dihydropyran? Possible Initiators of its Polymerisation?. <i>Macromolecular Chemistry and Physics</i> , 2003, 204, 2099-2104.	1.1	7
1268	1H,13C,17O NMR and quantum-chemical study of the stereochemistry of the sulfoxide and sulfone derivatives of 3-arylidene-1-thioflavan-4-one epoxides. <i>Magnetic Resonance in Chemistry</i> , 2003, 41, 193-201.	1.1	38
1269	Dianionen von Tetraboranen(4): gefaltete aromatische Vierringe und ihre Reaktionen unter Erhaltung der Aromatizität. <i>Angewandte Chemie</i> , 2003, 115, 1758-1760.	1.6	20
1271	Triboracyclobutanide: viergliedrige Zweielektronen-Aromaten mit fluktuierenden Ger1/4st-Bindungen. <i>Angewandte Chemie</i> , 2003, 115, 693-695.	1.6	9
1272	Ein Diboracyclopropan mit planar-tetrakoordiniertem Kohlenstoffatom und ein Triborabicyclobutan. <i>Angewandte Chemie</i> , 2003, 115, 695-698.	1.6	7
1273	Topomerisierung eines verzerrt-rautenförmigen Tetraborans(4) und seine Hydroborierung zu einem closo-Pentaboran(7) mit nido-Struktur. <i>Angewandte Chemie</i> , 2003, 115, 1079-1082.	1.6	8
1274	Vibrational and Quantum-Chemical Study of Push-Pull Chromophores for Second-Order Nonlinear Optics from Rigidified Thiophene-Based π -Conjugating Spacers. <i>Chemistry - A European Journal</i> , 2003, 9, 3670-3682.	1.7	57
1275	Preparation, Structure, and Unique Thermal [2+2], [4+2], and [3+2] Cycloaddition Reactions of 4-Vinylideneoxazolidin-2-one. <i>Chemistry - A European Journal</i> , 2003, 9, 2419-2438.	1.7	60
1276	Facial Selectivity of the (R)-1,3-Dimethyl-1-Cyclohexyl Cation in the Gas Phase. <i>Chemistry - A European Journal</i> , 2003, 9, 5396-5403.	1.7	3
1277	Enhanced Li+ Binding Energies in Alkylbenzene Derivatives: The Scorpion Effect. <i>Chemistry - A European Journal</i> , 2003, 9, 4330-4338.	1.7	28
1278	The Open-Chain Trioxide CF3OC(O)OOC(O)OCF3. <i>Chemistry - A European Journal</i> , 2003, 9, 5135-5141.	1.7	22
1279	Computational Assessment of the Electronic Structure of 1-Azacyclohexa-2,3,5-triene (3 $\hat{2}$ -1H-Pyridine) and Its Benzo Derivative (3 $\hat{2}$ -1H-Quinoline) as well as Generation and Interception of 1-Methyl-3 $\hat{2}$ -1H-quinoline. <i>Chemistry - A European Journal</i> , 2003, 9, 4641-4649.	1.7	17

#	ARTICLE	IF	CITATIONS
1280	Theoretical Investigation of the Photochemical C2-C6Cyclisation of Enyne-Heteroallenes. Chemistry - A European Journal, 2003, 9, 4670-4677.	1.7	11
1281	Carâ€Parrinello Molecular Dynamics Study of the Rearrangement of the Valeramide Radical Cation. Chemistry - A European Journal, 2003, 9, 4396-4404.	1.7	8
1282	Substituent Effects on Oï£H Bond Dissociation Enthalpies and Ionization Potentials of Catechols: A DFT Study and Its Implications in the Rational Design of Phenolic Antioxidants and Elucidation of Structureâ€Activity Relationships for Flavonoid Antioxidants. Chemistry - A European Journal, 2003, 9, 502-508.	1.7	204
1283	Side-On Bridging Coordination of N2: Spectroscopic Characterization of the Planar Zr2N2 Core and Theoretical Investigation of Its Butterfly Distortion. Chemistry - A European Journal, 2003, 9, 520-530.	1.7	29
1284	Structural Investigation of a High-Affinity MnII Binding Site in the Hammerhead Ribozyme by EPR Spectroscopy and DFT Calculations. Effects of Neomycin B on Metal-Ion Binding. ChemBioChem, 2003, 4, 1057-1065.	1.3	54
1285	Dianions of Tetraboranes(4): Puckered Aromatic Four-Membered Rings and Their Reactions with Conservation of Aromaticity. Angewandte Chemie - International Edition, 2003, 42, 1717-1719.	7.2	44
1286	Breaking Down Barriers: The Liaison Between Sigmatropic Shifts, Electrocyclic Reactions, and Three-Center Cations. Angewandte Chemie - International Edition, 2003, 42, 5877-5882.	7.2	20
1287	Triboracyclobutanides: Four-Membered Two-Electron Aromatic Compounds with Fluctuating Skeletal Bonds. Angewandte Chemie - International Edition, 2003, 42, 669-671.	7.2	19
1288	A Diboracyclopropane with a Planar-Tetracoordinate Carbon Atom and a Triborabicyclobutane. Angewandte Chemie - International Edition, 2003, 42, 671-674.	7.2	29
1289	Topomerization of a Distorted Diamond-Shaped Tetraborane(4) and Its Hydroboration to a closo-Pentaborane(7) with a nido Structure. Angewandte Chemie - International Edition, 2003, 42, 1049-1052.	7.2	11
1290	A computational study on CunNO,Â±1 (n=1â€4) clusters by density functional methods. Chemical Physics, 2003, 294, 211-220.	0.9	12
1291	Low energy electron attachment to CH3CN. Chemical Physics Letters, 2003, 381, 216-222.	1.2	43
1292	Proton transfer between C20(OH)2 molecules: an ab initio study. Chemical Physics Letters, 2003, 368, 224-229.	1.2	3
1293	Geometries and electronic properties of AunPdm (n=1â€4, m=â~1, 0, 1) clusters. Chemical Physics Letters, 2003, 368, 153-161.	1.2	24
1294	A time-dependent density-functional theory investigation of the fluorescence behavior of related cyano and di-cyano isomers of 4-(N,N-dimethylamino) benzonitrile. Chemical Physics Letters, 2003, 368, 561-567.	1.2	15
1295	Ab initio correlated comparative study of the torsional potentials for 2,2â€2-bipyrrole and 2,2â€2-bifuran five membered heterocyclic dimers. Chemical Physics Letters, 2003, 369, 114-124.	1.2	24
1296	Theoretical study on PbS, PbO and their anions. Chemical Physics Letters, 2003, 370, 39-43.	1.2	21
1297	Gradient expansions in density functional calculations of intermolecular potentials. Chemical Physics Letters, 2003, 370, 353-359.	1.2	3

#	ARTICLE	IF	CITATIONS
1298	Density functional study of W2 and W3 clusters. <i>Chemical Physics Letters</i> , 2003, 370, 510-514.	1.2	24
1299	Gas phase photoisomerization of urocanic acid – a theoretical study. <i>Chemical Physics Letters</i> , 2003, 370, 625-630.	1.2	10
1300	Potential energy surface of aluminum and tungsten dimers. <i>Chemical Physics Letters</i> , 2003, 371, 35-39.	1.2	11
1301	Density functional theory and ab initio direct dynamics study on the reaction of $\text{BCl}_3 + \text{H}^+ \rightarrow \text{BCl}_2 + \text{HCl}$. <i>Chemical Physics Letters</i> , 2003, 373, 1-7.	1.2	4
1302	Theoretical study of hydrolysis reactions of tetravalent thorium ion. <i>Chemical Physics Letters</i> , 2003, 373, 213-217.	1.2	8
1303	Theoretical study of role of H ₂ O molecule on initial stage of reduction of O ₂ molecule in active site of cytochrome c oxidase. <i>Chemical Physics Letters</i> , 2003, 374, 45-52.	1.2	24
1304	Comparative study of dehydrogenation of methanol at Pt(111)/water and Pt(111)/vacuum interfaces. <i>Chemical Physics Letters</i> , 2003, 377, 236-242.	1.2	58
1305	Fundamental properties of small molecule models of Fe-only hydrogenase: computations relative to the definition of an entatic state in the active site. <i>Coordination Chemistry Reviews</i> , 2003, 238-239, 255-266.	9.5	186
1306	S ⁺ H proton dissociation enthalpies of thiophenolic cation radicals: a DFT study. <i>Computational and Theoretical Chemistry</i> , 2003, 663, 167-174.	1.5	42
1307	Theoretical study of spectroscopic constants and molecular properties of diatomic anions using B3LYP method. <i>Computational and Theoretical Chemistry</i> , 2003, 640, 183-189.	1.5	4
1308	Electro-oxidation of CO on Pt-based electrodes simulated by electronic structure calculations. <i>Journal of Electroanalytical Chemistry</i> , 2003, 554-555, 459-465.	1.9	18
1309	Guaiazulene-based phenolic radical scavengers: synthesis, properties, and EPR studies of their reaction with oxygen-centred radicals. <i>Tetrahedron</i> , 2003, 59, 5003-5018.	1.0	8
1310	Carbon-chain isomerization during the electrochemical fluorination in anhydrous hydrogen fluoride – a mechanistic study. <i>Journal of Fluorine Chemistry</i> , 2003, 124, 21-37.	0.9	22
1311	Vibrational study of push-pull chromophores for second-order non-linear optics derived from rigidified thiophene π -conjugating spacers. <i>Journal of Molecular Structure</i> , 2003, 651-653, 151-158.	1.8	34
1312	Theoretical description of the Raman spectrum of a vinylene-bridged quaterthiophene oligomer. <i>Journal of Molecular Structure</i> , 2003, 651-653, 657-664.	1.8	9
1313	UV-Vis, IR, Raman and theoretical characterization of a novel quinoid oligothiophene molecular material. <i>Journal of Molecular Structure</i> , 2003, 651-653, 665-673.	1.8	10
1314	Vibrational properties of [33](1,3,5)-cyclophane and bridged-hexaprismane. <i>Journal of Molecular Structure</i> , 2003, 655, 351-359.	1.8	4
1315	Structural characterization of two novel potential anticholinesterasic agents. <i>Journal of Molecular Structure</i> , 2003, 657, 191-198.	1.8	10

#	ARTICLE	IF	CITATIONS
1316	The chemical shift tensor of silylenes. <i>Journal of Organometallic Chemistry</i> , 2003, 686, 251-256.	0.8	38
1317	Theoretical study of the molecular structure for zirconium complexes. <i>Ceramics International</i> , 2003, 29, 471-475.	2.3	11
1318	A theoretical investigation of Ge_nSn ($n=1\text{--}4$) clusters. <i>Computational and Theoretical Chemistry</i> , 2003, 624, 257-265.	1.5	14
1319	Conformation of protonated trans-N-benzylideneaniline: a revisit. <i>Computational and Theoretical Chemistry</i> , 2003, 634, 311-314.	1.5	7
1320	A density functional investigation of Ag_nSn ($n=1\text{--}5$) clusters. <i>Computational and Theoretical Chemistry</i> , 2003, 635, 25-35.	1.5	16
1321	DFT studies on the molecular orbitals and related properties of $[\text{Ru}(\text{phen})_2(9,9\text{-}\lambda^2\text{-}2\text{R-dppq})]^{2+}$ ($\text{R}=\text{NH}_2, \text{OH}, \text{H}$). <i>Theoretical Chemistry Accounts</i> , 2003, 112, 1074-1081.	1.3	16
1322	Nucleus-independent chemical shift evaluation for benzo- and dibenzo-fused pyrrole, furan and thiophene derivatives. <i>Computational and Theoretical Chemistry</i> , 2003, 638, 157-162.	1.5	29
1323	Theoretical study of the molecular properties of methyl azidoformate and ethyl azidoformate. <i>Computational and Theoretical Chemistry</i> , 2003, 639, 109-115.	1.5	3
1324	A theoretical investigation on electronic properties and stability of Ir_xSix ($x=1\text{--}6$) clusters. <i>Chemical Physics</i> , 2003, 286, 181-192.	0.9	66
1325	Finding the global minima of clusters with non-empirical models: a comparison of results. <i>Chemical Physics</i> , 2003, 290, 279-295.	0.9	6
1326	Investigation of the molecular structure of radical cation of s-trioxane: quantum chemical calculations and low-temperature EPR results. <i>Radiation Physics and Chemistry</i> , 2003, 67, 237-241.	1.4	9
1327	Reduction of Cu(II) in matrix-assisted laser desorption/ionization mass spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2003, 14, 42-50.	1.2	62
1328	Metastable states of dimethyloxonium, $(\text{CH}_3)_2\text{OH}^+$. <i>International Journal of Mass Spectrometry</i> , 2003, 222, 49-61.	0.7	20
1329	Gas-phase basicity and enantiodiscrimination of some phosphorous-containing α -amino acid mimics. <i>International Journal of Mass Spectrometry</i> , 2003, 228, 349-358.	0.7	16
1330	On gaseous $\text{C}_4\text{H}_6\text{O}_2$ compounds in the atmosphere: new insights from collision experiments of the protonated molecules in the laboratory and on aircraft. <i>International Journal of Mass Spectrometry</i> , 2003, 228, 35-47.	0.7	5
1331	Protonation and methylation of thiophenol, thioanisole and their halogenated derivatives: mass spectrometric and computational study. <i>International Journal of Mass Spectrometry</i> , 2003, 228, 151-165.	0.7	12
1332	DFT investigation of copper-peptide complexes related to the octarepeat domain of the prion protein. <i>Inorganic Chemistry Communication</i> , 2003, 6, 650-653.	1.8	20
1333	The hybrid DF/HF calculations for the NS, NO, NN and ONS bridged radicals. <i>Crystal Engineering</i> , 2003, 6, 31-42.	0.7	1

#	ARTICLE	IF	CITATIONS
1334	Structural properties and ¹³ C chemical shifts of bis- and tris(2-thienyl)methinium and related cations: a combined theoretical and experimental study. <i>Journal of Physical Organic Chemistry</i> , 2003, 16, 53-62.	0.9	5
1335	Geometric and electronic structure of zwitterionic push-pull polyenes for nonlinear optics. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 303-310.	1.0	24
1336	Adiabatic connection approach to density functional theory of electronic systems. <i>International Journal of Quantum Chemistry</i> , 2003, 93, 166-190.	1.0	87
1337	Production and fragmentation of multiply charged ions in "electron-free" matrix-assisted laser desorption/ionization. <i>Rapid Communications in Mass Spectrometry</i> , 2003, 17, 2343-2348.	0.7	51
1338	Direct dynamics study of hydrogen abstraction using density functional theory: reaction. <i>Chemical Physics</i> , 2003, 286, 173-180.	0.9	7
1339	The origin of luminescence accompanying electrochemical reduction or chemical decomposition of peroxydisulfates. <i>Journal of Luminescence</i> , 2003, 105, 27-34.	1.5	44
1340	A theoretical study of the dioxygen activation by glucose oxidase and copper amine oxidase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2003, 1647, 173-178.	1.1	33
1341	DFT Calculations and Spectral Measurements of Charge-Transfer Complexes Formed by Aromatic Amines and Nitrogen Heterocycles with Tetracyanoethylene and Chloranil. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8939-8948.	1.1	66
1342	Full configuration interaction potential energy curves for breaking bonds to hydrogen: An assessment of single-reference correlation methods. <i>Journal of Chemical Physics</i> , 2003, 118, 1610-1619.	1.2	115
1343	Conformations of Benzene- and Dibenzo[a,l]pyrene Diol Epoxides Studied by Density Functional Theory: Ground States, Transition States, Dynamics, and Solvent Effects. <i>Chemical Research in Toxicology</i> , 2003, 16, 590-597.	1.7	6
1344	Nitrogen-enhanced negative bias temperature instability: An insight by experiment and first-principle calculations. <i>Applied Physics Letters</i> , 2003, 82, 1881-1883.	1.5	66
1345	Decarboxylation of carbonyloxy radicals: a density functional study. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 3891-3896.	1.3	10
1346	Interaction of Li ⁺ , Na ⁺ , and K ⁺ with the Proline Amino Acid. Complexation Modes, Potential Energy Profiles, and Metal Ion Affinities. <i>Journal of Physical Chemistry B</i> , 2003, 107, 2588-2594.	1.2	103
1347	First Identification of an Aliphatic cis- $\hat{\pm}$, $\hat{\pm}$ -Dinitroso Compound: A Combined Experimental and Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6731-6737.	1.1	7
1348	Aromaticity of Square Planar N4 ²⁻ in the M2N4 (M = Li, Na, K, Rb, or Cs) Species. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2882-2889.	1.1	49
1349	Long-range charge-transfer excited states in time-dependent density functional theory require non-local exchange. <i>Journal of Chemical Physics</i> , 2003, 119, 2943-2946.	1.2	1,416
1350	Theoretical Calculation of Accurate Absolute and Relative Gas- and Liquid-Phase O-H Bond Dissociation Enthalpies of 2-Mono- and 2,6-Disubstituted Phenols, Using DFT/B3LYP. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8594-8606.	1.1	74
1351	Origins of Opposite Absolute Stereoselectivities in Proline-Catalyzed Direct Mannich and Aldol Reactions. <i>Organic Letters</i> , 2003, 5, 1249-1251.	2.4	154

#	ARTICLE	IF	CITATIONS
1352	DENSITY FUNCTIONAL STUDIES OF Iridium CATALYZED ALKANE DEHYDROGENATION. <i>Advances in Inorganic Chemistry</i> , 2003, , 321-349.	0.4	8
1353	Lactam Hydrolysis Catalyzed by Mononuclear Metallo- β -lactamases: A Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2003, 107, 2366-2375.	1.2	29
1354	Catalytic Gas Phase Oxidation of Methanol to Formaldehyde. <i>Journal of the American Chemical Society</i> , 2003, 125, 3384-3396.	6.6	228
1355	Ab initio study of the polymer molecules (TeO ₂) as model systems for the local structure in TeO ₂ glass. <i>Physical Review B</i> , 2003, 68, .	1.1	24
1356	Raman, Infrared, and Surface-Enhanced Raman Spectroscopy in Combination with ab Initio and Density Functional Theory Calculations on 10-Isopropyl-10H-phenothiazine-5-oxide. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1811-1818.	1.1	40
1357	Hydrogen and Oxygen Adsorption on Rh _n (n = 1-6) Clusters. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10370-10380.	1.1	30
1358	Theoretical and Electrochemical Study of the Quinone-Benzoic Acid Adduct Linked by Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11161-11168.	1.1	29
1359	Modeling the Reaction Mechanisms of the Amide Hydrolysis in an N-(o-Carboxybenzoyl)-l-amino Acid. <i>Journal of the American Chemical Society</i> , 2003, 125, 6994-7000.	6.6	37
1360	Theoretical Study of the Reactivity of Fe ⁺ toward OCS. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8955-8960.	1.1	18
1361	Modifying Electronic Communication in Dimolybdenum Units by Linkage Isomers of Bridged Oxamidate Dianions. <i>Journal of the American Chemical Society</i> , 2003, 125, 13564-13575.	6.6	102
1362	Mn(III)-Based Oxidative Free-Radical Cyclizations of Substituted Allyl α -Methyl- β -ketoesters: Syntheses, DFT Calculations, and Mechanistic Studies. <i>Journal of Organic Chemistry</i> , 2003, 68, 2771-2778.	1.7	22
1363	Analytic and Variational χ^2 in the Slater-Roothaan Method. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10082-10089.	1.1	18
1364	Polyunsaturated Dicarboxylate Tethers Connecting Dimolybdenum Redox and Chromophoric Centers: Absorption Spectra and Electronic Structures. <i>Journal of the American Chemical Society</i> , 2003, 125, 5486-5492.	6.6	71
1365	Density Analysis of Intermolecular Orbital-Interaction Effects on the Second Hyperpolarizabilities of π - π Stacking Dimers. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4157-4164.	1.1	13
1366	Theoretical Studies of the Complex [(BPMEN)Fe(II)(NCCH ₃) ₂] ²⁺ , Precursor of Non-Heme Iron Catalysts for Olefin Epoxidation and Cis-Dihydroxylation. <i>Inorganic Chemistry</i> , 2003, 42, 8449-8455.	1.9	30
1367	Self-Assembled Oligo(phenylene-ethynylene) Molecular Electronic Switch Monolayers on Gold: Structures and Chemical Stability. <i>Langmuir</i> , 2003, 19, 8245-8255.	1.6	144
1368	Pyruvate Formate Lyase: A New Perspective. <i>Journal of Physical Chemistry B</i> , 2003, 107, 5751-5757.	1.2	16
1369	Comprehensive Model for the Electronic Structures of 1,2,4-Cyclohexatriene and Related Compounds. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11223-11230.	1.1	15

#	ARTICLE	IF	CITATIONS
1370	Agostic vs π -Interactions in Complexes of Ethynylsilanes and Ethynylgermanes with Cu ⁺ in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1370-1376.	1.1	37
1371	Kinetics of Reactions of Cl Atoms with Ethane, Chloroethane, and 1,1-Dichloroethane. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6565-6573.	1.1	43
1372	A Theoretical Rationalization of the Asymmetric Induction in Sulfinyl-Directed [5C + 2C] Intramolecular Cycloadditions. <i>Journal of Organic Chemistry</i> , 2003, 68, 9780-9786.	1.7	18
1373	Computational Study of the Halogen Atom π -Benzene Complexes. <i>Journal of the American Chemical Society</i> , 2003, 125, 8390-8399.	6.6	43
1374	Substituent Effects on Enthalpies of Formation: Δ Benzene Derivatives. <i>Journal of Physical Chemistry A</i> , 2003, 107, 366-371.	1.1	21
1375	Effects of the ancillary ligands of polypyridyl ruthenium(ii) complexes on the DNA-binding behaviors. <i>New Journal of Chemistry</i> , 2003, 27, 1255.	1.4	133
1376	The Reactions of Imidazol-2-ylidenes with the Hydrogen Atom: Δ A Theoretical Study and Experimental Confirmation with Muonium. <i>Journal of the American Chemical Society</i> , 2003, 125, 11565-11570.	6.6	56
1377	On the Existence of Electronic States Confined by Charged Groups in Proteins. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1692-1697.	1.2	13
1378	Twofold Hydrogen Bridges as Observed in Amide-Templated Rotaxanes. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9634-9640.	1.1	20
1379	Cyclic Polyamidato Dianions as Bridges between Mo ²⁺ Units: Δ Synthesis, Crystal Structures, Electrochemistry, Absorption Spectra, and Electronic Structures. <i>Journal of the American Chemical Society</i> , 2003, 125, 8900-8910.	6.6	46
1380	Density Functional Theory Study of the Intramolecular [2 + 3] Cycloaddition of Azide to Nitriles. <i>Journal of Organic Chemistry</i> , 2003, 68, 9076-9080.	1.7	36
1381	Probing the Intrinsic Electronic Structure of the Cubane [4Fe μ -4S] Cluster: Δ Nature's Favorite Cluster for Electron Transfer and Storage. <i>Journal of the American Chemical Society</i> , 2003, 125, 14072-14081.	6.6	74
1382	The Trapping of the OH Radical by Coenzyme Q. A Theoretical and Experimental Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9712-9723.	1.1	17
1383	A Computational Study of the Mechanism for the Transmetalation of 2-Trimethylstannylbuta-1,3-diene with SnCl ₄ . <i>Journal of Organic Chemistry</i> , 2003, 68, 2673-2679.	1.7	4
1384	Experimental and theoretical study on DNA-binding and photocleavage properties of chiral complexes P^n - and L^n -[Ru(bpy) ₂ L] (L = o-hpip, m-hpip and p-hpip) Electronic supplementary information (ESI) available: electronic spectra and photocleavage diagrams. See http://www.rsc.org/suppdata/dt/b2/b212443b/ . <i>Dalton Transactions</i> , 2003, , 1352-1359.	1.6	102
1385	Density Functional Study on the Effect of the trans Axial Ligand of B ₁₂ Cofactors on the Heterolytic Cleavage of the Co π -C Bond. <i>Journal of Physical Chemistry B</i> , 2003, 107, 306-315.	1.2	48
1386	Transition Metal Mediated Epoxidation as Test Case for the Performance of Different Density Functionals: Δ A Computational Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5466-5471.	1.1	51
1387	Quantum Chemical Study of Zirconium Oxide Deposition on the Si(100) π (2 \times 1) Surface. <i>Journal of Physical Chemistry B</i> , 2003, 107, 9319-9324.	1.2	31

#	ARTICLE	IF	CITATIONS
1388	Selectivity of Metallocene-Catalyzed Olefin Polymerization: A Combined Experimental and Quantum Mechanical Study. Theansa-Me ₂ Si(Ind) ₂ Zr andansa-Me ₂ C(Cp)(Flu)Zr Systems. <i>Macromolecules</i> , 2003, 36, 8171-8177.	2.2	34
1389	Direct ab Initio Dynamics Study of the Reaction of the Hydrogen Atom with Formyl Chloride. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10435-10440.	1.1	5
1390	Transition Structures, Energetics, and Secondary Kinetic Isotope Effects for Cope Rearrangements of cis-1,2-Divinylcyclobutane and cis-1,2-Divinylcyclopropane: A DFT Study. <i>Journal of Organic Chemistry</i> , 2003, 68, 9635-9642.	1.7	43
1391	The Arsenic Fluorides AsFn (n = 1-6) and Their Anions: Structures, Thermochemistry, and Electron Affinities. <i>Journal of Physical Chemistry A</i> , 2003, 107, 258-266.	1.1	32
1392	Calculations of Site-Specific CO Stretching Frequencies for Copper Carbonyls with the Near Spectroscopic Accuracy: CO Interaction with Cu+/MFI. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10381-10388.	1.1	71
1393	Density Functional Study on the Mechanism of Bicyclic Guanidine-Catalyzed Strecker Reaction. <i>Journal of Organic Chemistry</i> , 2003, 68, 8786-8789.	1.7	52
1394	Spectroscopic and Theoretical Study of Push-Pull Chromophores Containing Thiophene-Based Quinonoid Structures as Electron Spacers. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12175-12183.	1.2	40
1395	Double C(sp ³) dehydrogenation as a route to coordinated Arduengo carbenes: experiment and computation on comparative C-acidity. <i>New Journal of Chemistry</i> , 2003, 27, 1446-1450.	1.4	36
1396	Gas-Phase Potassium Binding Energies of MALDI Matrices: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6891-6900.	1.1	14
1397	Naphthalenyl, Anthracenyl, Tetracenyl, and Pentacenyl Radicals and Their Anions. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6311-6316.	1.1	16
1398	Theoretical Study of [N ₃ X] ⁺ (X = O, S, Se, Te) Systems. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5561-5565.	1.1	11
1399	Kinetics of the Unimolecular Decomposition of the C ₂ Cl ₃ Radical. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6574-6579.	1.1	13
1400	Photophysical Characterization of Fluorescent DNA Base Analogue, tC. <i>Journal of Physical Chemistry B</i> , 2003, 107, 9094-9101.	1.2	71
1401	Theoretical Characterization of Oxoanion, XO _m ⁿ⁻ , Solvation. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5778-5788.	1.1	34
1402	Theoretical Investigation of the Reaction of Co ⁺ with OCS. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8618-8622.	1.1	19
1403	Chemical and Photochemical Electron Transfer of New Helianthrone Derivatives: Aspects of Their Photodynamic Activity. <i>Journal of the American Chemical Society</i> , 2003, 125, 1376-1384.	6.6	38
1404	Combined Quantum Chemistry and Photoelectron Spectroscopy Study of the Electronic Structure and Reduction Potentials of Rubredoxin Redox Site Analogues. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2898-2907.	1.1	39
1405	On the Origin of Higher Rotational Barriers in Thioamides than in Amides. Remote Substituent Effects on the Conformational Stability of the Thioamide Group in Thioacetanilides. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5854-5861.	1.1	26

#	ARTICLE	IF	CITATIONS
1406	UV Raman Spectrum of 1,3-Dimethylcyclopentenyl Cation Adsorbed in Zeolite H-MFI. <i>Journal of the American Chemical Society</i> , 2003, 125, 866-867.	6.6	22
1407	Structures of Hydrated Oxygen Anion Clusters: DFT Calculations for O-(H ₂ O) _n , O ₂ -(H ₂ O) _n , and O ₃ -(H ₂ O) _n (n= 0-4). <i>Journal of Physical Chemistry A</i> , 2003, 107, 962-967.	1.1	26
1408	Cage-like Si ₁₂ clusters with endohedral Cu, Mo, and W metal atom impurities. <i>Physical Review B</i> , 2003, 67, .	1.1	87
1409	Optimized effective potential made simple: Orbital functionals, orbital shifts, and the exact Kohn-Sham exchange potential. <i>Physical Review B</i> , 2003, 68, .	1.1	162
1410	Proximity effects on semiconducting mineral surfaces II. <i>Geochimica Et Cosmochimica Acta</i> , 2003, 67, 941-953.	1.6	39
1411	The structure of hematite (α-Fe ₂ O ₃) (001) surfaces in aqueous media: scanning tunneling microscopy and resonant tunneling calculations of coexisting O and Fe terminations. <i>Geochimica Et Cosmochimica Acta</i> , 2003, 67, 985-1000.	1.6	125
1412	Hydrogen isotope exchange kinetics between H ₂ O and H ₄ SiO ₄ from ab initio calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2003, 67, 1259-1276.	1.6	20
1413	Surface structure effects on direct reduction of iron oxides by <i>Shewanella oneidensis</i> . <i>Geochimica Et Cosmochimica Acta</i> , 2003, 67, 4489-4503.	1.6	76
1414	Elementary reaction path on polychlorinated biphenyls formation from polychlorinated benzenes in heterogeneous phase using ab initio molecular orbital calculation. <i>Chemosphere</i> , 2003, 50, 457-467.	4.2	5
1415	Solvation Effects on Alternative Nucleophilic Substitution Reaction Paths for Chloride/Allyl Chloride and ¹³ C-Methylated Congeners. <i>Journal of Organic Chemistry</i> , 2003, 68, 6375-6386.	1.7	30
1416	Modeling the Reaction Mechanisms of the Imide Formation in an N-(o-Carboxybenzoyl)-l-amino Acid. <i>Journal of the American Chemical Society</i> , 2003, 125, 3642-3648.	6.6	17
1417	Nitro-Functionalized Oligothiophenes as a Novel Type of Electroactive Molecular Material: Spectroscopic, Electrochemical, and Computational Study. <i>Journal of the American Chemical Society</i> , 2003, 125, 2524-2534.	6.6	106
1418	Kinetic Study and Theoretical Analysis of Hydroxyl Radical Trapping and Spin Adduct Decay of Alkoxy-carbonyl and Dialkoxyphosphoryl Nitrones in Aqueous Media. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4407-4414.	1.1	80
1419	The Joint Use of Catastrophe Theory and Electron Localization Function to Characterize Molecular Mechanisms. A Density Functional Study of the Diels-Alder Reaction between Ethylene and 1,3-Butadiene. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6014-6024.	1.1	149
1420	Effects of ligand planarity on the interaction of polypyridyl Ru(II) complexes with DNA. <i>Dalton Transactions</i> , 2003, , 2260.	1.6	185
1421	The Adenine-Thymine Base Pair Radical Anion: Adding an Electron Results in a Major Structural Change. <i>Journal of Physical Chemistry B</i> , 2003, 107, 848-853.	1.2	106
1422	Theoretical Prediction of the Co-C Bond Strength in Cobalamins. <i>Journal of Physical Chemistry A</i> , 2003, 107, 7539-7545.	1.1	168
1423	Isodesmic Reactions for Transition States: Reactions of Cl Atoms with Methane and Halogenated Methanes. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11082-11091.	1.1	20

#	ARTICLE	IF	CITATIONS
1424	X-ray Structures, Photophysical Characterization, and Computational Analysis of Geometrically Constrained Copper(I)-Phenanthroline Complexes. <i>Inorganic Chemistry</i> , 2003, 42, 4918-4929.	1.9	28
1425	Trends in Cyclopentadienyl Main-Group-Metal Bonding. <i>Organometallics</i> , 2003, 22, 1562-1576.	1.1	120
1426	Anion photoelectron spectroscopy of solvated transition state precursors. <i>Journal of Chemical Physics</i> , 2003, 119, 872-879.	1.2	18
1427	Energetics and Structures of Adamantane and the 1- and 2-Adamantyl Radicals, Cations, and Anions. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9479-9485.	1.1	37
1428	Antioxidant Activity of Bakuchiol: Experimental Evidences and Theoretical Treatments on the Possible Involvement of the Terpenoid Chain. <i>Chemical Research in Toxicology</i> , 2003, 16, 1062-1069.	1.7	57
1429	Density-functional investigation on the mechanism of H-atom abstraction by lipoxygenase. <i>Journal of Biological Inorganic Chemistry</i> , 2003, 8, 294-305.	1.1	119
1430	Study of Local Hard-Soft Acid-Base Principle: Effects of Basis Set, Electron Correlation, and the Electron Partitioning Method. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5755-5762.	1.1	24
1431	Kinetics of the Reaction of the CCl ₂ Biradical with Molecular Chlorine. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10292-10295.	1.1	5
1432	Thermodynamic properties (S ₂₉₈ , Cp(T), internal rotations and group additivity parameters) in vinyl and phenyl hydroperoxides. Electronic supplementary information (ESI) available: Internal rotation barriers, Fourier expansion coefficients for internal rotation potentials for vinyl and phenyl hydroperoxides. See http://www.rsc.org/suppdata/cp/b2/b207030h/ . <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 300-307.	1.3	13
1433	1,2-Chlorine atom migration in 3-chloro-2-butyl radicals: a computational study. Electronic supplementary information (ESI) available: Calculated energies and enthalpies of stationary points, full structural information, and structures of trans-but-2-ene (9) and trans-but-2-ene radical (10). See http://www.rsc.org/suppdata/ob/b2/b209981k/ . <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 168-172.	1.5	12
1434	σ-Donor olefin substituents alter olefin binding to CpFe(CO) ₂ ⁺ . <i>New Journal of Chemistry</i> , 2003, 27, 1769-1774.	1.4	19
1435	Quantum chemical studies of redox-active enzymes. <i>Faraday Discussions</i> , 2003, 124, 289.	1.6	50
1436	Unusual flexibility of 2,5-bis(4-pyridylethynyl)thiophene self-assembled with Co(NCS) ₂ in a novel coordination polymer. <i>Chemical Communications</i> , 2003, , 2528.	2.2	24
1437	Spin trapping by bis(benzene)chromium: A density functional study. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 1337.	1.3	14
1438	Reactivity of the tetraphenyldithioimidodiphosphine-diiodine (HLA ₂) adduct towards indium powder. <i>Dalton Transactions</i> , 2003, , 1515-1519.	1.6	13
1439	An Assessment of Theoretical Methods for the Calculation of Accurate Structures and SN Bond Dissociation Energies of S-Nitrosothiols (RSNOs). <i>Journal of Physical Chemistry A</i> , 2003, 107, 9946-9952.	1.1	57
1440	A direct optimization method for calculating density functionals and exchange-correlation potentials from electron densities. <i>Journal of Chemical Physics</i> , 2003, 118, 2498.	1.2	267
1441	Theoretical calculations of effective exchange integrals by spin projected and unprojected broken-symmetry methods. I. Cluster models of K ₂ NiF ₄ -type solids. <i>Journal of Chemical Physics</i> , 2003, 118, 9747-9761.	1.2	27

#	ARTICLE	IF	CITATIONS
1442	Quantum states of hydrogen transfer and vibration in malonaldehyde. <i>Molecular Physics</i> , 2003, 101, 3263-3276.	0.8	43
1443	The influence of hydrogen bonding interactions on the C-H bond activation step in class I ribonucleotide reductases. Electronic supplementary information (ESI) available: Energies and structures of stationary points for studied reactions. See http://www.rsc.org/suppdata/ob/b2/b210536p/ . <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 692-699.	1.5	23
1444	Density Functionals for Non-relativistic Coulomb Systems in the New Century. <i>Lecture Notes in Physics</i> , 2003, , 1-55.	0.3	96
1445	Quantum-Chemical Dynamics with the Slater-Roothaan Method. <i>Theoretical and Computational Chemistry</i> , 2003, , 111-124.	0.2	0
1446	DENSITY FUNCTIONAL STUDY OF SELECTED MONO-ZINC AND GEM-DIZINC RADICAL CARBENOID CYCLOPROPANATION REACTIONS: OBSERVATION OF AN EFFICIENT RADICAL ZINC CARBENOID CYCLOPROPANATION REACTION AND THE INFLUENCE OF THE LEAVING GROUP ON RING CLOSURE. <i>Journal of Theoretical and Computational Chemistry</i> , 2003, 02, 357-369.	1.8	6
1447	Spin Distribution in Dehydrogenated Coniferyl Alcohol and Associated Dilignol Radicals. <i>Holzforschung</i> , 2003, 57, 59-61.	0.9	19
1448	Formation of β^2 -O-4 Lignin Models -A Theoretical Study. <i>Holzforschung</i> , 2003, 57, 466-478.	0.9	35
1449	A Density Functional Theory Study of Coniferyl Alcohol Intermonomeric Cross Linkages in Lignin - Three-Dimensional Structures, Stabilities and the Thermodynamic Control Hypothesis. <i>Holzforschung</i> , 2003, 57, 150-164.	0.9	31
1450	Algorithm to derive exact exchange-correlation potentials from correlated densities in atoms. <i>Physical Review A</i> , 2003, 67, .	1.0	50
1451	III: PROPERTIES OF COMPLEX SYSTEMS. <i>Molecular Physics</i> , 2003, 101, 211-225.	0.8	11
1452	Observation of a HI leaving group following ultraviolet photolysis of CH ₂ I ₂ in water and anab initio investigation of the O-H insertion/HI elimination reactions of the CH ₂ I isopolyhalomethane species with H ₂ O and 2H ₂ O. <i>Journal of Chemical Physics</i> , 2003, 119, 4671-4681.	1.2	17
1453	Metal and ligand hyperfine couplings in transition metal complexes: The effect of spin-orbit coupling as studied by coupled perturbed Kohn-Sham theory. <i>Journal of Chemical Physics</i> , 2003, 118, 3939-3948.	1.2	354
1454	Why is Al ₁₁ B ₂ not a magic number in TOF-MS?. <i>Journal of Chemical Physics</i> , 2003, 119, 5949-5954.	1.2	12
1455	Resonant nonlinear polarizabilities in the time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2003, 119, 8809-8823.	1.2	142
1456	Study of negative-bias temperature-instability-induced defects using first-principle approach. <i>Applied Physics Letters</i> , 2003, 83, 3063-3065.	1.5	9
1457	Polarizability of water clusters: Anab initio investigation. <i>Journal of Chemical Physics</i> , 2003, 118, 8547-8550.	1.2	42
1458	Ab initio direct dynamics studies on the reactions of H atoms with CH ₃ Cl and CH ₃ Br. <i>Journal of Chemical Physics</i> , 2003, 118, 4920-4928.	1.2	5
1459	Restricted density-functional linear response theory calculations of electronic g-tensors. <i>Journal of Chemical Physics</i> , 2003, 119, 10489-10496.	1.2	26

#	ARTICLE	IF	CITATIONS
1460	Indium phosphide (001)-(2Å-1): Direct evidence for a hydrogen-stabilized surface reconstruction. <i>Physical Review B</i> , 2003, 68, .	1.1	16
1461	The accuracy of density functionals for electric field gradients. Test calculations for ScX, CuX and GaX (X=F, Cl, Br, I, H and Li). <i>Journal of Chemical Physics</i> , 2003, 119, 5988-5994.	1.2	45
1462	Linear relationship between H+-trapping reaction energy and defect generation: Insight into nitrogen-enhanced negative bias temperature instability. <i>Applied Physics Letters</i> , 2003, 83, 530-532.	1.5	22
1463	Connections between second-order Green's function theory and many-body perturbation approaches in density functional theory. <i>Journal of Chemical Physics</i> , 2003, 118, 461-470.	1.2	28
1464	A statistical, ab initio, quantum mechanical study of the photolysis and final state distributions of singlet ketene. <i>Journal of Chemical Physics</i> , 2003, 119, 6003-6016.	1.2	14
1465	Local hybrid functionals based on exact-expression approximate exchange. <i>Journal of Chemical Physics</i> , 2003, 118, 8576-8583.	1.2	23
1466	Quantum Monte Carlo investigations of density functional theory of the strongly inhomogeneous electron gas. <i>Physical Review B</i> , 2003, 68, .	1.1	20
1467	A theoretical study on the stability of N15+ cluster. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 1116-1122.	1.3	6
1468	On the electronic structures of gaseous transition metal halide complexes, FeX4 and MX3 (M=Mn, Fe, Co, Ni, Cu, Zn, Cd, Hg). <i>Journal of Chemical Physics</i> , 2003, 119, 8311-8320.	1.2	48
1469	Mechanism of electron localization at edge-sharing units in amorphous SiO2. <i>Physical Review B</i> , 2003, 68, .	1.1	8
1470	Ab initio periodic approach to electronic structure and magnetic exchange in A2CuO2X2 (A=Ca, Sr). <i>Physical Review B</i> , 2003, 68, .	1.1	10
1471	ALGEBRAIC EQUATION AND ITERATIVE OPTIMIZATION FOR THE OPTIMIZED EFFECTIVE POTENTIAL IN DENSITY FUNCTIONAL THEORY. <i>Journal of Theoretical and Computational Chemistry</i> , 2003, 02, 627-638.	1.8	82
1472	THEORETICAL PREDICTION OF POTENTIAL ENERGY SURFACE FOR N14 CLUSTER. <i>Journal of Theoretical and Computational Chemistry</i> , 2003, 02, 7-14.	1.8	8
1473	THE DISSOCIATION AND ISOMERIZATION REACTIONS OF N11 ISOMERS. <i>Journal of Theoretical and Computational Chemistry</i> , 2003, 02, 15-22.	1.8	1
1474	Non-linear optical anomalies near the phase transitions in polysiloxane chromophore incorporated within an oligoetheracrylate photopolymer matrix. <i>Journal of Optics</i> , 2003, 5, 87-90.	1.5	4
1475	Gas-phase reactivity of lactones: structure and stability of their Cu+ complexes. <i>Molecular Physics</i> , 2003, 101, 1249-1258.	0.8	7
1476	Computational Studies on the Mechanism of Orotidine Monophosphate Decarboxylase. <i>Advances in Physical Organic Chemistry</i> , 2003, 38, 183-218.	0.5	3
1477	Quantum Chemical Investigation of Spin-Forbidden Transitions in Dithiosuccinimide. <i>Zeitschrift Fur Physikalische Chemie</i> , 2003, 217, 205-230.	1.4	5

#	ARTICLE	IF	CITATIONS
1478	Is Allylphosphine a Carbon or a Phosphorus Base in the Gas Phase?. <i>European Journal of Mass Spectrometry</i> , 2003, 9, 245-255.	0.5	5
1479	Stereochemical Interactions in Ammonium Dications, Hypervalent Diammonium Cation-Radicals and Ammonium Radicals. A B3-MP2 Computational Study. <i>European Journal of Mass Spectrometry</i> , 2003, 9, 267-277.	0.5	5
1480	Theoretical Study on the Structures and Absorption Properties of Yellow Azomethine Dyes. <i>Bulletin of the Chemical Society of Japan</i> , 2003, 76, 733-742.	2.0	6
1481	DFT Study for CO and H ₂ ; Adsorption and Related Reactions on Pt alloy Electrode. <i>Electrochemistry</i> , 2004, 72, 865-869.	0.6	0
1482	Theoretical study on Fe-Al clusters: geometric structure, bonding law and electronic structures *. <i>Progress in Natural Science: Materials International</i> , 2004, 14, 675-680.	1.8	0
1483	Ab initio theory of magnetic interactions at surfaces. <i>Journal of Physics Condensed Matter</i> , 2004, 16, S2557-S2574.	0.7	11
1484	Change of magnetic properties of benzenes in multiple-decked sandwich clusters: Mn(C ₆ H ₆) _{n+1} (n = 1-5). <i>Journal of Physics Condensed Matter</i> , 2004, 16, S2557-S2574.	0.7	5
1485	Spin Polarization of a Multiple-decked Sandwich Clusters: M(C ₆ H ₆) ₂ (M = Mn, Fe, Co). <i>Journal of the Physical Society of Japan</i> , 2004, 73, 2292-2295.	0.7	10
1486	Density-functional study of lanthanum, ytterbium, and lutetium dimers. <i>Physical Review A</i> , 2004, 69, .	1.0	20
1487	How O ₂ Binds to Heme. <i>Journal of Biological Chemistry</i> , 2004, 279, 14561-14569.	1.6	170
1488	The ability of silylenes to bind excess electrons: Electron affinities of SiX ₂ , and SiXY species (X,Y=H,CH ₃ ,SiH ₃ ,F,Cl,Br). <i>Journal of Chemical Physics</i> , 2004, 121, 9361-9367.	1.2	14
1489	Structural stability and electronic state of transition metal trimers. <i>Journal of Chemical Physics</i> , 2004, 121, 4699-4704.	1.2	13
1490	Static dipole polarizability and binding energy of sodium clusters Na _n (n=1-10): A critical assessment of all-electron based post Hartree-Fock and density functional methods. <i>Journal of Chemical Physics</i> , 2004, 120, 6487-6494.	1.2	58
1491	Adsorption of 3-pyrroline on Si(100) from first principles. <i>Journal of Chemical Physics</i> , 2004, 120, 9745-9751.	1.2	9
1492	Aqua dissociation nature of cesium hydroxide. <i>Journal of Chemical Physics</i> , 2004, 121, 204.	1.2	29
1493	Fragmentation and deformation mechanism of glycine isomers in gas phase: Investigations of charge effect. <i>Journal of Chemical Physics</i> , 2004, 120, 11600-11614.	1.2	9
1494	Performance of the \bar{I}_n -dependent functionals in predicting the magnetic coupling of ionic antiferromagnetic insulators. <i>Journal of Chemical Physics</i> , 2004, 120, 3811-3816.	1.2	50
1495	An ab initio calculation of the anisotropic hyperfine coupling constants in the low-lying vibronic levels of the $X^2\Sigma^+$ electronic state of CCCH. <i>Journal of Chemical Physics</i> , 2004, 121, 12361.	1.2	6

#	ARTICLE	IF	CITATIONS
1496	X-ray photoelectron spectroscopy of nitromethane adsorption products on Si(100): A model for Na ϵ 1s core-level shifts in silicon oxynitride films. <i>Journal of Applied Physics</i> , 2004, 95, 1963-1968.	1.1	40
1497	Substituent and ring effects on enthalpies of formation: 2-methyl- and 2-ethylbenzimidazoles versus benzene- and imidazole-derivatives. <i>Molecular Physics</i> , 2004, 102, 711-721.	0.8	16
1498	Directab initiodynamics study on the rate constants and kinetics isotope effects of CH ₃ O+H α †'CH ₂ O+H ₂ reaction. <i>Journal of Chemical Physics</i> , 2004, 121, 9474-9480.	1.2	9
1499	Complete structural and magnetic characterization of biological radicals in solution by an integrated quantum mechanical approach: Glycyl radical as a case study. <i>Journal of Chemical Physics</i> , 2004, 121, 6710-6718.	1.2	65
1500	The impact of the self-interaction error on the density functional theory description of dissociating radical cations: Ionic and covalent dissociation limits. <i>Journal of Chemical Physics</i> , 2004, 120, 524-539.	1.2	141
1501	Recent Developments in Computational Bioinorganic Chemistry. <i>Structure and Bonding</i> , 2004, , 37-70.	1.0	15
1502	Exchange and correlation as a functional of the local density of states. <i>Physical Review B</i> , 2004, 69, .	1.1	5
1503	An ab initio study of the hyperfine structure in the X α €Š[sup 2] electronic state of CCCH. <i>Journal of Chemical Physics</i> , 2004, 121, 2636.	1.2	8
1504	Theoretical calculations of effective exchange integrals by spin projected and unprojected broken-symmetry methods. III. Cluster models of three-dimensional KNiF ₃ solid. <i>Journal of Chemical Physics</i> , 2004, 121, 2199-2207.	1.2	5
1505	Reference-state one-particle density-matrix theory. <i>Physical Review A</i> , 2004, 69, .	1.0	3
1506	Magic clusters MAu ₄ (M=Ti and Zr) and their dimers: How magic are they?. <i>Journal of Chemical Physics</i> , 2004, 120, 11363-11366.	1.2	23
1507	A search for a strong physisorption site for H[sub 2] in Li-doped porous carbons. <i>Journal of Chemical Physics</i> , 2004, 121, 12548.	1.2	31
1508	Reaction mechanism of ZrCl/sub 4/ with Ge/Si[100]-(2 x 1): a density functional theory study of initial stage of ZrO/sub 2/ atomic layer deposition on SiGe alloy surface. , 0, , .		0
1509	First Principles Studies of Metal-Oxide Surfaces. <i>Topics in Catalysis</i> , 2004, 28, 59-69.	1.3	41
1510	The germanium clusters Ge _n (n= 1â€“6) and their anions: structures, thermochemistry and electron affinities. <i>Molecular Physics</i> , 2004, 102, 579-598.	0.8	33
1511	Low-Temperature Decomposition of Hydrogen Sulfide under the Conditions of Conjugate Chemisorption and Catalysis. <i>Doklady Physical Chemistry</i> , 2004, 399, 283-286.	0.2	14
1512	Docking and scoring of metallo- β -lactamases inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , 2004, 18, 287-302.	1.3	29
1513	Preparation and structure of an unexpected dehydrogenation product from 2,6-diphenylcyclohexanone oxime. <i>Journal of Chemical Crystallography</i> , 2004, 34, 103-110.	0.5	2

#	ARTICLE	IF	CITATIONS
1514	A Quantum Chemical Study of the Molecular Structure of Active Centers and Growth in Ethylene Polymerization in the Catalytic System LFeCl ₂ /AlMe ₃ (L = 2,6-Bis-Iminopyridyl). <i>Kinetics and Catalysis</i> , 2004, 45, 508-518.	0.3	2
1515	Dissociative Adsorption of Water Molecules on Uncharged Surfaces of Indium(111) and Gallium. <i>Russian Journal of Electrochemistry</i> , 2004, 40, 379-386.	0.3	6
1516	Dissociation chemistry of hydrogen halides in water. <i>Journal of Chemical Physics</i> , 2004, 120, 9524-9535.	1.2	117
1517	[3 + 2] Cycloreversion of Bicyclo[m.3.0]alkan-3-on-2-yl-1-oxonium Ylides to Alkenyloxyketenes. Stereospecific Aspect. <i>Journal of Organic Chemistry</i> , 2004, 69, 1331-1336.	1.7	21
1518	Spectroscopic and computational characterization of the nickel-containing F430 cofactor of methyl-coenzyme M reductase. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 77-89.	1.1	26
1519	The catalytic cycle of catechol oxidase. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 577-590.	1.1	54
1520	First principle calculations of ¹¹³ Cd chemical shifts for proteins and model systems. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 591-599.	1.1	35
1521	Diels-Alder reactivity of benzannulated isobenzofurans as assessed by density functional theory. <i>Journal of Molecular Modeling</i> , 2004, 10, 87-93.	0.8	10
1522	A computational approach to the synthesis of dirithromycin. <i>Journal of Molecular Modeling</i> , 2004, 10, 94-101.	0.8	3
1523	IR optical limiting in europium and thulium doped oxide glasses. <i>Infrared Physics and Technology</i> , 2004, 45, 253-263.	1.3	17
1524	Enantiopure stereoisomeric homologues of glutamic acid: chemoenzymatic synthesis and assignment of their absolute configurations. <i>Tetrahedron: Asymmetry</i> , 2004, 15, 3079-3090.	1.8	22
1525	X-Ray Study of the Electronic Structure of Copper(II) Acetylacetonate. <i>Journal of Structural Chemistry</i> , 2004, 45, 800-807.	0.3	7
1526	Influence of molecular structure on the C-N bond strength in the nitroalkane series: II. Nitroethane, fluoronitroethanes, chloronitroethanes, and fluorochloronitroethanes. <i>Russian Journal of General Chemistry</i> , 2004, 74, 1708-1713.	0.3	3
1527	Mechanism of gas-phase decomposition of nitroethylene: A theoretical study. <i>Russian Journal of General Chemistry</i> , 2004, 74, 1227-1242.	0.3	8
1528	Influence of arene-arene interactions on the conformation of acyclic molecules: ¹ H NMR and dipole moment experimental results. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 71-82.	0.9	5
1529	Tuning carbanion reactivity by complexing with boranes: ¹³ C-elimination reaction as a model. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 983-989.	0.9	0
1530	Generation and characterization of ionic and neutral methylene isothiocyanate by a combined tandem mass spectrometry and computational study. <i>Rapid Communications in Mass Spectrometry</i> , 2004, 18, 1939-1946.	0.7	4
1531	Polynitrogen clusters containing five-membered rings. <i>International Journal of Quantum Chemistry</i> , 2004, 97, 933-943.	1.0	8

#	ARTICLE	IF	CITATIONS
1532	Periodic approach to the electronic structure and magnetic coupling in $KCuF_3$, K_2CuF_4 , and $Sr_2CuO_2Cl_2$ low-dimensional magnetic systems. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 805-823.	1.0	36
1533	Spectroscopic constants and molecular properties of $CN^?$, $SiH^?$, $PO^?$, $SO^?$, $SF^?$, and $SiS^?$: Density functional study. <i>International Journal of Quantum Chemistry</i> , 2004, 98, 447-455.	1.0	10
1534	Theoretical investigation of the structures and properties of fluoromethyl peroxy radicals. <i>International Journal of Quantum Chemistry</i> , 2004, 98, 502-514.	1.0	4
1535	Theoretical studies on effective exchange integrals using spin correlation function analysis and magnetic effective density functional (MEDF) method. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 927-936.	1.0	3
1536	Kinetic and Thermodynamic Control by Chemical Bond Rearrangement on a Si(001) Surface. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 1349-1352.	7.2	22
1537	Peptide-Biphenyl Hybrids as Calpain Inhibitors. <i>Chemistry and Biodiversity</i> , 2004, 1, 442-457.	1.0	16
1538	Theoretical Explorations of Enantioselective Alkylation Reactions of Pyrroles and Indoles Organocatalyzed by Chiral Imidazolidinones. <i>Advanced Synthesis and Catalysis</i> , 2004, 346, 1175-1185.	2.1	91
1540	η^1 -Pbasal Coordination of P_4X_3 ($X = S, Se$) Molecules toward 16e Ruthenium Fragments. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 293-300.	1.0	22
1541	Mechanism of Oxidation of (olefin)RhI and -IrI Complexes by H_2O_2 . <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 2385-2391.	1.0	23
1542	The Electronic Structure of (Diiminopyridine)cobalt(I) Complexes. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 1204-1211.	1.0	138
1543	First ICN Adduct with a Selenium Donor ($R = Se$): Is It an Ionic $[RSeCN]^+ + I^-$ or a π -Shaped $R(I)SeCN$ Hypervalent Compound?. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 2363-2368.	1.0	17
1544	$[Ni(C_4H_{13}N_3)_2]_3(Sb_3S_6)_2$: The First Structure Containing Isolated Heterocyclic $[Sb_3S_6]^{3-}$ Anions. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 2553-2556.	1.0	52
1545	Preparation, Structure Determination and Cytotoxicity of the PdII-Bleomycin A2 Complex. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 3118-3126.	1.0	1
1546	Syntheses and Reactions of a Stable 1,2-Dichloro-1,2-diborolane and Aromatic Tetraboranes. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 3063-3073.	1.0	33
1547	Reaction of Mercury(0) with the I2 Adduct of Tetraphenyldithioimidodiphosphinic Acid (SPPH2)2NH (HL) ? Crystal Structures of $[Hg(HL)_2]$ and HgI_2 . <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 4660-4668.	1.0	18
1548	A Comparison of Transition States During H-Atom Abstraction of Monophenols and Catechol by Methyl Radical. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 120-128.	1.2	10
1549	Hydrogen Migration Over Organic Tapes: [1,5] Sigmatropic Shiftamers. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 273-280.	1.2	6
1550	Computational Study on the Effects of Substituents and Functional Groups in the Isomerization of 1- and 2-Substituted Propenes, Acetaldimines, and Aldehydes. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 1432-1443.	1.2	13

#	ARTICLE	IF	CITATIONS
1551	Diastereoselective Synthesis of Thieno[3,2-c:4,5]cyclopenta[1,2-d][1,3]oxazolines $\hat{\alpha}$ New Ligands for the Copper-Catalyzed Asymmetric Conjugate Addition of Diethylzinc to Enones. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 4442-4451.	1.2	20
1552	Spectroscopic and Theoretical Study of the Molecular and Electronic Structures of a Terthiophene-Based Quinodimethane. <i>ChemPhysChem</i> , 2004, 5, 529-539.	1.0	46
1553	Synthesis, Characterization, and DNA-Binding Properties of the Ruthenium(II) Complexes [Ru(dipn)(dptp)](ClO ₄) ₂ and [Ru(dipn)(pat)](ClO ₄) ₂ (dipn=N-(3-Aminpropyl)propane-1,3-diamine; Tj ETQq0 0 0 rgBT /Overl 1180-1193.	1.0	27
1554	Direct dynamic study on the hydrogen abstraction reaction CH ₃ CN + OH \rightarrow CH ₂ CN + H ₂ O. <i>Journal of Computational Chemistry</i> , 2004, 25, 251-257.	1.5	10
1555	Systematic quantum chemical study of DNA-base tautomers. <i>Journal of Computational Chemistry</i> , 2004, 25, 83-99.	1.5	173
1556	Class I ribonucleotide reductase revisited: The effect of removing a proton on Glu441. <i>Journal of Computational Chemistry</i> , 2004, 25, 311-321.	1.5	31
1557	The arsenic clusters As _n (n = 1-5) and their anions: Structures, thermochemistry, and electron affinities. <i>Journal of Computational Chemistry</i> , 2004, 25, 907-920.	1.5	40
1558	Quantitative structure-activity relationships for phenyl triazolinones of protoporphyrinogen oxidase inhibitors: A density functional theory study. <i>Journal of Computational Chemistry</i> , 2004, 25, 1827-1832.	1.5	27
1559	Near-infrared Fourier transform surface-enhanced Raman scattering spectroscopy of 1,4-benzodiazepine drugs employing gold films over nanospheres. <i>Journal of Raman Spectroscopy</i> , 2004, 35, 368-383.	1.2	16
1560	Differences in retention of dioxin-like compounds and organochlorinated insecticides on an immunochromatographic column. Interpretation and applicability. <i>Journal of Separation Science</i> , 2004, 27, 1093-1101.	1.3	6
1561	A DFT Quantum-Chemical Study of the Structure of Precursors and Active Sites of Catalyst Based on 2,6-Bis(imino)pyridyl Fe(II) Complexes. <i>Macromolecular Theory and Simulations</i> , 2004, 13, 583-591.	0.6	12
1562	Computational Approaches to Activity in Rhodium-Catalysed Hydroformylation. <i>Chemistry - A European Journal</i> , 2004, 10, 2435-2444.	1.7	48
1563	Vibrational and Quantum-Chemical Study of Nonlinear Optical Chromophores Containing Dithienothiophene as the Electron Relay. <i>Chemistry - A European Journal</i> , 2004, 10, 3805-3816.	1.7	44
1564	Computational Investigation of Hydrogen Abstraction from 2-Aminoethanol by the 1,5-Dideoxyribose-5-yl Radical: A Model Study of a Reaction Occurring in the Active Site of Ethanolamine Ammonia Lyase. <i>Chemistry - A European Journal</i> , 2004, 10, 2781-2788.	1.7	10
1565	Synthesis and Determination of the Absolute Configuration of Fugomycin and Desoxyfugomycin: CD Spectroscopy and Fungicidal Activity of Butenolides. <i>Chemistry - A European Journal</i> , 2004, 10, 4584-4593.	1.7	31
1566	Understanding the Molecular Mechanism of the 1,3-Dipolar Cycloaddition between Fulminic Acid and Acetylene in Terms of the Electron Localization Function and Catastrophe Theory. <i>Chemistry - A European Journal</i> , 2004, 10, 5165-5172.	1.7	95
1567	Theory and Experiment in Concert: Templated Synthesis of Amide Rotaxanes, Catenanes, and Knots. <i>Chemistry - A European Journal</i> , 2004, 10, 4777-4789.	1.7	62
1568	Vinyl Sulfoxides as Stereochemical Controllers in Intermolecular Pauson-Khand Reactions: Applications to the Enantioselective Synthesis of Natural Cyclopentanoids. <i>Chemistry - A European Journal</i> , 2004, 10, 5443-5459.	1.7	41

#	ARTICLE	IF	CITATIONS
1569	Experimental and theoretical investigation on the correlation between aqueous precursors structure and crystalline phases of zirconia. <i>Journal of Molecular Structure</i> , 2004, 690, 181-187.	1.8	21
1570	8-Aryl substituted boron-dipyrromethene dyes: crystal structures and computational studies. <i>Journal of Molecular Structure</i> , 2004, 697, 29-40.	1.8	11
1571	A DFT-based QSARs study of protoporphyrinogen oxidase inhibitors: phenyl triazolinones. <i>Bioorganic and Medicinal Chemistry</i> , 2004, 12, 6183-6191.	1.4	34
1572	Carbon-hydrogen and carbon-heteroatom bond activation using iridium(II) complexes. <i>Inorganica Chimica Acta</i> , 2004, 357, 2863-2869.	1.2	17
1573	Secondary kinetic isotope effects in cation-bound dimers of acetone (C ₃ H ₆ O) ₂ with M = H, Li, Na, K, Rb, Ag, and Cs. <i>International Journal of Mass Spectrometry</i> , 2004, 233, 103-109.	0.7	28
1574	Generation and characterization of ionic and neutral selenocumulene HC ₃ Se ⁺ by tandem mass spectrometry and computational study. <i>International Journal of Mass Spectrometry</i> , 2004, 232, 231-237.	0.7	5
1575	Composition and structure of activated complexes in stereoselective deprotonation of cyclohexene oxide by a mixed dimer of chiral lithium amide and lithiated imidazole. <i>Tetrahedron: Asymmetry</i> , 2004, 15, 1607-1613.	1.8	14
1576	Theoretical study of O ₂ adsorption on GaN surfaces. <i>Computational and Theoretical Chemistry</i> , 2004, 668, 51-55.	1.5	15
1577	Quantum chemical DFT and spectroscopic study of a push-pull chromophore for second-order nonlinear optics containing bithiophene as the electron relay. <i>Computational and Theoretical Chemistry</i> , 2004, 709, 187-193.	1.5	27
1578	Theoretical elucidation of structure-activity relationship for coumarins to scavenge peroxy radical. <i>Computational and Theoretical Chemistry</i> , 2004, 673, 199-202.	1.5	36
1579	Ab initio direct dynamics studies of the hydrogen abstraction on the reaction of Cl with CHBrF ₂ . <i>Computational and Theoretical Chemistry</i> , 2004, 674, 23-27.	1.5	6
1580	Ground state of lutetium dimer by density functional methods. <i>Computational and Theoretical Chemistry</i> , 2004, 677, 55-58.	1.5	1
1581	Electronic structures of hafnium dimer and trimer by density functional theory. <i>Computational and Theoretical Chemistry</i> , 2004, 680, 1-4.	1.5	8
1582	Density functional theory kinetic assessment of hydrogen abstraction from hydrocarbons by O ₂ . <i>Computational and Theoretical Chemistry</i> , 2004, 681, 89-98.	1.5	7
1583	Ab initio study for the hydrogen abstraction reaction C ₂ H ₅ +H ⁺ C ₂ H ₄ +H ₂ . <i>Computational and Theoretical Chemistry</i> , 2004, 682, 163-170.	1.5	7
1584	NICS evaluation for Cope rearrangements of cis-1,2-divinylcyclopropane and cis-1,2-divinylcyclobutane. <i>Computational and Theoretical Chemistry</i> , 2004, 681, 113-116.	1.5	9
1585	Electronic structures, DNA-binding and related properties of complexes [Ru(bpy) ₂ L] ₂ ⁺ (L=ip, pip, hpip). <i>Computational and Theoretical Chemistry</i> , 2004, 682, 225-233.	1.5	35
1586	Direct DFT dynamics study of the addition reaction CF ₂ CHF+H ⁺ product. <i>Computational and Theoretical Chemistry</i> , 2004, 685, 147-154.	1.5	2

#	ARTICLE	IF	CITATIONS
1587	Insight into the stability and structural properties of HPS3 isomers from density functional theory computations. <i>Computational and Theoretical Chemistry</i> , 2004, 712, 1-7.	1.5	0
1588	Comparative parametric method 5 (PM5) study of trans-stilbene. <i>Computational and Theoretical Chemistry</i> , 2004, 686, 103-108.	1.5	10
1589	Implications of hyperconjugative effects on bond lengths of allylic systems. An NBO investigation. <i>Computational and Theoretical Chemistry</i> , 2004, 710, 105-110.	1.5	9
1590	Energy of the O–NO ₂ bond dissociation and the mechanism of the gas-phase monomolecular decomposition of aliphatic alcohol nitroesters. <i>Computational and Theoretical Chemistry</i> , 2004, 686, 185-192.	1.5	16
1591	NMR and inelastic incoherent neutron scattering (IINS) studies of monohydroxy-17 and -21-substituted derivatives of progesterone. <i>Solid State Nuclear Magnetic Resonance</i> , 2004, 25, 21-27.	1.5	6
1592	Surface reaction mechanisms for atomic layer deposition of silicon nitride. <i>Surface Science</i> , 2004, 557, 159-170.	0.8	34
1593	On the geometric structure of the (0001) hematite surface. <i>Surface Science</i> , 2004, 558, 4-14.	0.8	48
1594	Quantum chemical study of surface reactions of glycine on the Si(100)-2 \times 1 surface. <i>Surface Science</i> , 2004, 569, 12-22.	0.8	30
1595	Unusual reversal of regioselectivity in antibody-mediated aldol additions with unsymmetrical methyl ketones. <i>Tetrahedron</i> , 2004, 60, 619-632.	1.0	25
1596	Selectivities in the 1,3-dipolar cycloaddition of nitrile oxides to dicyclopentadiene and its derivatives. <i>Tetrahedron</i> , 2004, 60, 1453-1462.	1.0	28
1597	Electronic effects on the interactions of complexes [Ru(phen) ₂ (p-L)] ²⁺ (L=MOPIP, HPIP, and NPIP) with DNA. <i>Inorganica Chimica Acta</i> , 2004, 357, 285-293.	1.2	64
1598	Synthesis and reactivity of new methylallylpalladium(II) complexes with bidentate 2-(methylthio-N-benzylidene)anilines. <i>Journal of Organometallic Chemistry</i> , 2004, 689, 395-404.	0.8	4
1599	Electronic excitation spectra and singlet–triplet coupling in psoralen and its sulfur and selenium analogs. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2004, 167, 201-212.	2.0	21
1600	Effects of the substitution positions of Br group in intercalative ligand on the DNA-binding behaviors of Ru(II) polypyridyl complexes. <i>Journal of Inorganic Biochemistry</i> , 2004, 98, 87-97.	1.5	61
1601	Carbon monoxide MgO from dispersed solids to single crystals: a review and new advances. <i>Progress in Surface Science</i> , 2004, 76, 71-146.	3.8	207
1602	Fourier transform infrared and Raman spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2004, 60, 2171-2180.	2.0	16
1603	Modeling deoxyribose radicals by neutralization-reionization mass spectrometry. Part 1. Preparation, dissociations, and energetics of 2-hydroxyoxolan-2-yl radical, neutral isomers, and cations. <i>Journal of the American Society for Mass Spectrometry</i> , 2004, 15, 1055-1067.	1.2	7
1604	Modeling deoxyribose radicals by neutralization-reionization mass spectrometry. Part 2. Preparation, dissociations, and energetics of 3-hydroxyoxolan-3-yl radical and cation. <i>Journal of the American Society for Mass Spectrometry</i> , 2004, 15, 1068-1079.	1.2	5

#	ARTICLE	IF	CITATIONS
1605	Reaction of hydroquinone with hematite. <i>Journal of Colloid and Interface Science</i> , 2004, 274, 442-450.	5.0	24
1606	Reduced activation energy and crystalline size for yttria-stabilized zirconia nano-crystals. <i>Journal of Crystal Growth</i> , 2004, 267, 100-109.	0.7	38
1607	The fate of nitric oxide in its reaction with the 14-valence-electron planar species [(tBu ₂ PCH ₂ SiMe ₂) ₂ N]RuCl. <i>Journal of Molecular Catalysis A</i> , 2004, 224, 51-59.	4.8	8
1608	Molecular structure of the complex of hexano-6-lactam with calcium bromide. <i>European Polymer Journal</i> , 2004, 40, 1423-1431.	2.6	1
1609	A novel perchlorate-bridged tetranuclear zinc(II) structure with tris(2-aminoethyl)amine ligand. <i>Inorganic Chemistry Communication</i> , 2004, 7, 906-908.	1.8	10
1610	Infrared absorption, Raman, and SERS investigations in conjunction with theoretical simulations on a phenothiazine derivative. <i>Chemical Physics</i> , 2004, 298, 87-95.	0.9	27
1611	Correlation between the energy and electron density representations of reactivity: mPW1K study of the asymmetric S _N 2 reactions at the saturated nitrogen. <i>Chemical Physics</i> , 2004, 298, 125-134.	0.9	12
1612	FT-Raman, surface-enhanced Raman spectroscopy and theoretical investigations of diclofenac sodium. <i>Chemical Physics</i> , 2004, 298, 167-174.	0.9	37
1613	Prediction of novel complexation of porphine and BF ₃ : Is it a 1:1 or 1:2 species?. <i>Chemical Physics</i> , 2004, 301, 1-7.	0.9	11
1614	Tautomerism of 9-acridinamines substituted at the exocyclic nitrogen atom in view of computational predictions and experimental findings. <i>Chemical Physics</i> , 2004, 303, 301-308.	0.9	8
1615	A computational investigation on GenCl ⁿ⁺ and GenCl (n=1-6) clusters by density functional methods. <i>Chemical Physics</i> , 2004, 305, 253-258.	0.9	8
1616	A density functional study of EPR hyperfine coupling of vanadocene(IV) complexes. <i>Chemical Physics</i> , 2004, 305, 291-298.	0.9	18
1617	Addition of nucleophiles to the 9-cyano-10-methylacridinium cation: utilization in their chemiluminescent assay. <i>Analytica Chimica Acta</i> , 2004, 507, 229-236.	2.6	15
1618	Real time observation of trans-cis isomerization on azobenzene SAM induced by optical near field enhancement. <i>Applied Surface Science</i> , 2004, 228, 265-270.	3.1	19
1619	Density functional study of the second row transition metal dimers. <i>Chemical Physics Letters</i> , 2004, 383, 251-255.	1.2	38
1620	Predicting energies and geometries for reactions involved in atmosphere chemistry: a comparison study between hybrid DFT methods. <i>Chemical Physics Letters</i> , 2004, 384, 20-24.	1.2	31
1621	Construction of local hybrid exchange-correlation potentials and their evaluation for nuclear shielding constants. <i>Chemical Physics Letters</i> , 2004, 386, 8-16.	1.2	42
1622	Are hemispherical caps of boron nitride nanotubes possible?. <i>Chemical Physics Letters</i> , 2004, 386, 403-407.	1.2	47

#	ARTICLE	IF	CITATIONS
1623	A density functional theory study of n-doped 3,4-ethylenedioxythiophene oligomers. <i>Chemical Physics Letters</i> , 2004, 386, 408-413.	1.2	18
1624	Theoretical enthalpies of formation and O-H bond dissociation enthalpy of an Î±-tocopherol model and its free radical. <i>Chemical Physics Letters</i> , 2004, 388, 274-278.	1.2	12
1625	Time resolved resonance Raman studies on triplet excited state of 2-methoxy-naphthalene by photo-sensitization. <i>Chemical Physics Letters</i> , 2004, 390, 427-432.	1.2	6
1626	An ab initio study of the side chain of Nafion. <i>Chemical Physics Letters</i> , 2004, 389, 64-67.	1.2	20
1627	Unrestricted open-shell Kohn-Sham scheme with local hybrid exchange-correlation potentials: improved calculation of electronic g-tensors for transition-metal complexes. <i>Chemical Physics Letters</i> , 2004, 391, 16-21.	1.2	33
1628	A theoretical investigation on fullerene-like phosphorus clusters. <i>Chemical Physics Letters</i> , 2004, 396, 27-33.	1.2	29
1629	On the optimal value of Î± for the Hartree-Fock-Slater method. <i>Chemical Physics Letters</i> , 2004, 399, 417-421.	1.2	7
1630	A quantum chemical study of the water-assisted mechanism in one-carbon unit transfer reaction catalyzed by glycylamide ribonucleotide transformylase. <i>Biophysical Chemistry</i> , 2004, 110, 259-266.	1.5	8
1631	Evaluation of carbohydrate molecular mechanical force fields by quantum mechanical calculations. <i>Carbohydrate Research</i> , 2004, 339, 937-948.	1.1	61
1632	Stabilization of porous silicon surface by thermal decomposition of acetylene. <i>Applied Surface Science</i> , 2004, 225, 389-394.	3.1	147
1633	Atomic Modeling of Nitrogen Neighboring Effect on Negative Bias Temperature Instability of pMOSFETs. <i>IEEE Electron Device Letters</i> , 2004, 25, 504-506.	2.2	20
1634	Re-evaluation of the Mn(salen) mediated epoxidation of alkenes by means of the B3LYP* density functionalElectronic supplementary information (ESI) available: Optimised geometries, bonding energies, final gradients, spin expectation values, and imaginary frequencies for transition states. See http://www.rsc.org/suppdata/cp/b4/b402188f/ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 3747.	1.3	28
1635	Effect of the self-interaction error for three-electron bonds: On the development of new exchange-correlation functionals. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 1096-1112.	1.3	107
1636	Molecular and Electronic Structure in the Metal-to-Ligand Charge Transfer Excited States of fac-[Re(4,4'-X2bpy)(CO)3(4-Etpy)]+* (X = CH3, H, Co2Et). Application of Density Functional Theory and Time-Resolved Infrared Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3518-3526.	1.1	79
1637	Protonation effect on the electronic spectrum of tryptophan in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2633.	1.3	108
1638	Dissociation of acetone radical cation (CH3COCH3+Ë™ â†' CH3CO++CH3Ë™): An ab initio direct classical trajectory study. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 5166-5171.	1.3	21
1639	Theoretical investigations of structure and mechanism of the oxygen-evolving complex in PSII. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 4772.	1.3	84
1640	Validation of density functional methods for computing structures and energies of mercury(IV) complexesElectronic supplementary information (ESI) available: Structure of transition state for HgH4 dissociation and tables with CP-connections and transition state structures. See http://www.rsc.org/suppdata/cp/b3/b315019d/ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 1122.	1.3	55

#	ARTICLE	IF	CITATIONS
1641	Structures, thermochemistry, vibrational frequencies and integrated infrared intensities of SF ₅ CF ₃ and SF ₅ , with implications for global temperature patterns. <i>Molecular Physics</i> , 2004, 102, 1415-1439.	0.8	12
1642	PROTON AND ELECTRON TRANSFERS IN [NiFe] HYDROGENASE. <i>Advances in Inorganic Chemistry</i> , 2004, 56, 101-125.	0.4	56
1643	A self-consistent reaction field model of solvation using distributed multipoles. I. Energy and energy derivatives. <i>Journal of Chemical Physics</i> , 2004, 120, 2343-2350.	1.2	46
1644	Assessment of recently developed exchange-correlation functionals for the description of torsion potentials in π -conjugated molecules. <i>Journal of Chemical Physics</i> , 2004, 121, 3096-3101.	1.2	63
1645	Dissolution of a base (RbOH) by water clusters. <i>Journal of Chemical Physics</i> , 2004, 121, 4665-4670.	1.2	15
1646	Theoretical Enthalpies of Formation and O-H Bond Dissociation Enthalpy of an Ubiquinol Model and Its Free Radical. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2508-2513.	1.1	4
1647	Spectroscopic Properties and Electronic Structure of Pentammineruthenium(II) Dinitrogen Oxide and Corresponding Nitrosyl Complexes: A Binding Mode of N ₂ O and Reactivity. <i>Inorganic Chemistry</i> , 2004, 43, 6979-6994.	1.9	72
1648	A Theoretical Study of Divalent Lanthanide (Sm and Yb) Complexes with a Triazacyclononane-Functionalized Tetramethylcyclopentadienyl Ligand. <i>Organometallics</i> , 2004, 23, 1953-1960.	1.1	22
1649	Density Functional Theory Investigations on the Chemical Basis of the Selectivity Filter in the K ⁺ Channel Protein. <i>Journal of the American Chemical Society</i> , 2004, 126, 4711-4716.	6.6	26
1650	Theoretical Studies of Benzonitrile at the Si(100)-2 \times 1 Surface. <i>Journal of Physical Chemistry B</i> , 2004, 108, 8305-8310.	1.2	18
1651	Dominant Role of C-Br \cdots N Halogen Bond in Molecular Self-Organization. Crystallographic and Quantum-Chemical Study of Schiff-Base-Containing Triazoles. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12327-12332.	1.2	44
1652	Synthesis, Structure, and Dynamics of Molybdenum Imido Alkyne Complexes. <i>Organometallics</i> , 2004, 23, 4070-4076.	1.1	11
1653	Charge Separation and Charge Distribution in Rearrangement Reactions of $\dot{\text{I}}^2$ -(Phosphatoxy)alkyl Radicals. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2324-2331.	1.1	8
1654	Density Functional Theory Investigations of the Direct Oxidation of Methane on an Fe-Exchanged Zeolite. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4362-4368.	1.2	45
1655	Ab initio study of the hyperfine structure of the X ² Σ^+ electronic state of HCCS. <i>Molecular Physics</i> , 2004, 102, 2623-2634.	0.8	8
1656	DFT Analysis of Fe(H ₂ O) ₆ ³⁺ and Fe(H ₂ O) ₆ ²⁺ Structure and Vibrations; Implications for Isotope Fractionation. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2726-2732.	1.1	92
1657	Theoretical Study of the Trapping of the OOH Radical by Coenzyme Q. <i>Journal of the American Chemical Society</i> , 2004, 126, 920-927.	6.6	37
1658	Ab Initio Calculations of the Structures and Vibrational Spectra of Ethene Complexes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 146-156.	1.1	25

#	ARTICLE	IF	CITATIONS
1659	Charge-Transfer Induced Large Nonlinear Optical Properties of Small Al Clusters: Al_4M_4 ($M = Li, Na$). <i>Tj ETQq0.0.0 rgBT /Overlock 1</i>	1.1	68
1660	Ab Initio Molecular Orbital Investigation of a Precursor in Ethylene Biosynthesis: A Proton Transfer in a Cluster of 1-Aminocyclopropane-1-carboxylic Acid and Water. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5417-5423.	1.1	2
1661	Structural and Topological Characterization of the Three-Electron Bond: The SO Radicals. <i>Journal of Physical Chemistry A</i> , 2004, 108, 898-906.	1.1	46
1662	Mechanistic Insight into the Symmetric Fission of $[4Fe^{\sim}4S]$ Analogue Complexes and Implications for Cluster Conversions in Iron-Sulfur Proteins. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6750-6757.	1.1	24
1663	Mechanism of Trialkylborane Promoted Adhesion to Low Surface Energy Plastics. <i>Macromolecules</i> , 2004, 37, 7974-7978.	2.2	54
1664	Chloride-Triggered Disproportionation of a Mononuclear RhII(nbd) Species to RhI(nbd) and RhIII(1-norbornenyl) Complexes: Possibilities for Wacker Type Mono-oxygenation of Norbornadiene to Norbornenone. <i>Organometallics</i> , 2004, 23, 4236-4246.	1.1	27
1665	Density Functional Calculations on Class III Ribonucleotide Reductase: A Substrate Reaction Mechanism with Two Formates. <i>Journal of Physical Chemistry B</i> , 2004, 108, 2056-2065.	1.2	13
1666	Temperature-Dependent Kinetics of the Gas-Phase Reactions of OH with Cl ₂ , CH ₄ , and C ₃ H ₈ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 10464-10472.	1.1	38
1667	The Silicon Hydride Clusters Si ₃ H _n ($n = 8$) and Their Anions: Structures, Thermochemistry, and Electron Affinities. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11345-11353.	1.1	26
1668	Aromatic vs Diradical Character in the Transition States of the Cope Rearrangements of 1,5-Hexadiene and Its Cyano Derivatives. <i>Journal of Physical Chemistry A</i> , 2004, 108, 194-202.	1.1	25
1669	Reactivity Extrapolation from Small to Large Molecular Systems via Isodesmic Reactions for Transition States. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10714-10722.	1.1	9
1670	Performance of Density Functionals for Calculating Barrier Heights of Chemical Reactions Relevant to Astrophysics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7621-7636.	1.1	80
1671	Synthesis and Properties of Palladium Diselenolenes: X-ray Crystal Structures of $[Pd\{SeC(R_1)C(R_2)Se\}(PBU_3)_2]$ [$R_1, R_2 = (CH_2)_n, n = 4, 5, 6$]. <i>Inorganic Chemistry</i> , 2004, 43, 7101-7110.	1.9	14
1672	Modeling Substituent and Conformational Effects on the Reactivity of Antitumor Agents Containing a Cyclopropylcyclohexadienone Subunit. <i>Journal of Organic Chemistry</i> , 2004, 69, 6202-6213.	1.7	5
1673	Synthesis and Reactivity of the Hydrido- and Alkylrhenium Methylidene Complexes $Cp^*(PMe_3)_2(R)ReCH_2$ ($R = H, CH_3$). <i>Journal of the American Chemical Society</i> , 2004, 126, 14804-14815.	6.6	9
1674	CO/Ethene Copolymerization at Zirconocene Centers?. <i>Organometallics</i> , 2004, 23, 855-860.	1.1	8
1675	The triplet state of cytosine and its derivatives: Electron impact and quantum chemical study. <i>Journal of Chemical Physics</i> , 2004, 121, 11668-11674.	1.2	47
1676	Solution and Crystal Structures of Chiral Molecules Can Be Significantly Different: tert-Butylphenylphosphinoselenoic Acid. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2072-2079.	1.1	18

#	ARTICLE	IF	CITATIONS
1677	Characterization of 5-Hydroxy-8-oxo-7,8-dihydroguanosine in the Photosensitized Oxidation of 8-Oxo-7,8-dihydroguanosine and Its Rearrangement to Spiroiminodihydantoin. <i>Journal of the American Chemical Society</i> , 2004, 126, 16777-16782.	6.6	80
1678	Scanning Tunneling Microscopy and Theoretical Study of Competitive Reactions in the Dissociative Chemisorption of CCl ₄ on Iron Oxide Surfaces. <i>Journal of Physical Chemistry B</i> , 2004, 108, 16753-16760.	1.2	21
1679	Quantum Chemical Calculations of the NHA Bound Nitric Oxide Synthase Active Site: O ₂ Binding and Implications for the Catalytic Mechanism. <i>Journal of the American Chemical Society</i> , 2004, 126, 10267-10270.	6.6	18
1680	Chiroptical Properties of Organic Radical Cations. The Electronic and Vibrational Circular Dichroism Spectra of $\hat{I}\pm$ -Tocopherol Derivatives and Sterically Hindered Chiral Hydroquinone Ethers. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9540-9549.	1.1	14
1681	Defining Electronic Excited States Using Time-Resolved Infrared Spectroscopy and Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3527-3536.	1.1	96
1682	Hypervalency Avoided: A Simple Substituted BrF ₃ and BrF ₅ Molecules. Structures, Thermochemistry, and Electron Affinities of the Bromine Hydrogen Fluorides HBrF ₂ and HBrF ₄ . <i>Journal of the American Chemical Society</i> , 2004, 126, 14950-14959.	6.6	9
1683	Surface-Enhanced Raman Scattering and Density Functional Theoretical Study of Anthranil Adsorbed on Colloidal Silver Particles. <i>Journal of Physical Chemistry B</i> , 2004, 108, 17491-17496.	1.2	36
1684	Orbital Interactions in the Ruthenium Olefin Metathesis Catalysts. <i>Organometallics</i> , 2004, 23, 76-80.	1.1	107
1685	Quantum Dynamical Study of \hat{I}^2 -Hydrogen Transfer in Two Selected Late-Transition-Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11116-11126.	1.1	13
1686	Combined ab Initio Quantum Mechanics and Classical Molecular Dynamics Studies of Polyphosphazene Polymer Electrolytes: A Competitive Solvation of Li ⁺ and LiCF ₃ SO ₃ . <i>Journal of Physical Chemistry B</i> , 2004, 108, 15694-15702.	1.2	49
1687	The Resting State of P450cam: A QM/MM Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7468-7478.	1.2	67
1688	Aromatic vs Aliphatic C-H Cleavage of Alkyl-Substituted Pyridines by (PNiPr)Re Compounds. <i>Journal of the American Chemical Society</i> , 2004, 126, 2105-2113.	6.6	59
1689	Electronic Structures of MCO (M = Nb, Ta, Rh, Ir, Pd, Pt) Molecules by Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10906-10910.	1.1	13
1690	Transition Structures, Energetics, and Nucleus-Independent Chemical Shifts for $\hat{G}\hat{I}\hat{E}$ Electrocyclizations of Dienylketenes to Cyclohexadienones: A DFT Study. <i>Journal of Organic Chemistry</i> , 2004, 69, 1940-1947.	1.7	23
1691	Aspects of Aqueous Iron and Manganese (II/III) Self-Exchange Electron Transfer Reactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5242-5248.	1.1	27
1692	Optical Characterization of Oligo(phenylene-ethynylene) Self-Assembled Monolayers on Gold. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12547-12559.	1.2	62
1693	The Vinyl Radical and Fluorinated Vinyl Radicals, C ₂ H ₃ -nFn (n = 0-3), and Corresponding Anions: A Comparison with the Isoelectronic Complexes [X-A-YC ₂ Z] ⁻ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 1608-1615.	1.1	12
1694	The Spin Dependence of the Spatial Size of Fe(II) and of the Structure of Fe(II)-Porphyrins. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4653-4657.	1.1	36

#	ARTICLE	IF	CITATIONS
1695	Comparison between the Geometric and Electronic Structures and Reactivities of {FeNO}7 and {FeO}8 Complexes: A Density Functional Theory Study. <i>Journal of the American Chemical Society</i> , 2004, 126, 505-515.	6.6	93
1696	Computational Studies on the Electrocyclizations of 1-Amino-1,3,5-hexatrienes. <i>Journal of Organic Chemistry</i> , 2004, 69, 8024-8028.	1.7	34
1697	Silicon ⁺ Carbon Unsaturated Compounds. 67. Photolysis of cis- and trans-1,2-Dimethyl-1,2-diphenyl-1,2-disilacyclopentane. <i>Organometallics</i> , 2004, 23, 1509-1518.	1.1	4
1698	Thermochemical Properties, Rotation Barriers, Bond Energies, and Group Additivity for Vinyl, Phenyl, Ethynyl, and Allyl Peroxides. <i>Journal of Physical Chemistry A</i> , 2004, 108, 8353-8366.	1.1	60
1699	Singlet ⁺ Triplet Energy Gaps of Gas-Phase RNA and DNA Bases. A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6554-6561.	1.1	52
1700	Investigation of Transition Metal ⁺ Imido Bonding in M(NBut)2(dpma). <i>Inorganic Chemistry</i> , 2004, 43, 3605-3617.	1.9	36
1701	Novel Interhalogen Molecules: Structures, Thermochemistry, and Electron Affinities of Dibromine Fluorides Br2Fn/Br2Fn-(n= 1-6). <i>Journal of Physical Chemistry A</i> , 2004, 108, 3598-3614.	1.1	11
1702	Combined Raman and Computational Study of a Novel Series of Macrocyclic π -Conjugated Diacetylene-Bridged β -Linked Oligothiophenes. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3158-3167.	1.2	24
1703	Reaction Products of W(CO)6 with Formamidines; Electronic Structure of a W2($\frac{1}{4}$ -CO)2 Core with Unsymmetric Bridging Carbonyls. <i>Inorganic Chemistry</i> , 2004, 43, 6954-6964.	1.9	18
1704	Kinetics and Thermochemistry of the Reaction of 2-Chloroallyl Radicals with Molecular Oxygen. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11339-11344.	1.1	2
1705	Transition Structures, Energetics, and Nucleus-Independent Chemical Shifts for Divinylcyclobutene-to-Cyclooctatriene Rearrangement: A DFT Study. <i>Journal of Organic Chemistry</i> , 2004, 69, 857-862.	1.7	4
1706	Vibrational Stark Effects on Carbonyl, Nitrile, and Nitrosyl Compounds Including Heme Ligands, CO, CN, and NO, Studied with Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2004, 108, 6450-6457.	1.2	53
1707	Li intercalation in TiO2 anatase: Raman spectroscopy and lattice dynamic studies. <i>Journal of Chemical Physics</i> , 2004, 121, 2348-2355.	1.2	48
1708	Theoretical Study of Nitrogen-Rich BeN4 Compounds. <i>Journal of Physical Chemistry A</i> , 2004, 108, 665-670.	1.1	12
1709	Trifluoromethyl Chloroformate, ClC(O)OCF3: Structure, Conformation, and Vibrational Analysis Studied by Experimental and Theoretical Methods. <i>Journal of Physical Chemistry A</i> , 2004, 108, 699-706.	1.1	20
1710	Electron hole formation in acidic zeolite catalysts. <i>Journal of Chemical Physics</i> , 2004, 121, 6034-6041.	1.2	49
1711	Mixed nitrogen/oxygen ligand affinities for bipovalent metal ions and dioxygen binding to cobalt(ii) complexes. <i>Dalton Transactions</i> , 2004, , 1358.	1.6	12
1712	Charge Transport in DNA-Based Devices. <i>Topics in Current Chemistry</i> , 2004, , 183-228.	4.0	227

#	ARTICLE	IF	CITATIONS
1713	Hybrid Meta Density Functional Theory Methods for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions: The MPW1B95 and MPWB1K Models and Comparative Assessments for Hydrogen Bonding and van der Waals Interactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6908-6918.	1.1	1,497
1714	Ground and Low-Lying States of $\text{Cu}^{2+} \cdot \text{H}_2\text{O}$. A Difficult Case for Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6072-6078.	1.1	85
1715	Conformational Effects on the Optical Rotation of Alanine and Proline. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4269-4276.	1.1	103
1716	A Theoretical Study of the Mechanism for the Biogenesis of Cofactor Topaquinone in Copper Amine Oxidases. <i>Journal of the American Chemical Society</i> , 2004, 126, 3996-4006.	6.6	29
1717	Initiation of Electro-Oxidation of CO on Pt Based Electrodes at Full Coverage Conditions Simulated by Ab Initio Electronic Structure Calculations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 9888-9892.	1.2	16
1718	Making a Molecular Wire: Charge and Spin Transport through para-Phenylene Oligomers. <i>Journal of the American Chemical Society</i> , 2004, 126, 5577-5584.	6.6	372
1719	Electronic Modulation of Dithienothiophene (DTT) as π -Center of D- π -D Chromophores on Optical and Redox Properties: A Analysis by UV-Vis-NIR and Raman Spectroscopies Combined with Electrochemistry and Quantum Chemical DFT Calculations. <i>Journal of the American Chemical Society</i> , 2004, 126, 13363-13376.	6.6	52
1720	A Quantum Chemical Study of the Atomic Layer Deposition of Al_2O_3 Using AlCl_3 and H_2O as Precursors. <i>Journal of Physical Chemistry B</i> , 2004, 108, 5718-5725.	1.2	64
1721	Density functional calculations of the vibronic structure of electronic absorption spectra. <i>Journal of Chemical Physics</i> , 2004, 120, 3544-3554.	1.2	293
1722	DENSITY FUNCTIONAL THEORETICAL STUDY OF NITRATED POLYCYCLIC AROMATIC HYDROCARBONS. <i>Polycyclic Aromatic Compounds</i> , 2004, 24, 37-64.	1.4	33
1723	$\text{S}_{\text{N}}2$ vs. E_2 on quaternary centres: an application to the synthesis of enantiopure β , γ -2-amino acids. <i>Chemical Communications</i> , 2004, , 980-981.	2.2	47
1724	Development of density functionals for thermochemical kinetics. <i>Journal of Chemical Physics</i> , 2004, 121, 3405-3416.	1.2	1,380
1725	Computational Study on Hydroxybenzotriazoles as Reagents for Ester Hydrolysis. <i>Journal of Organic Chemistry</i> , 2004, 69, 8634-8642.	1.7	41
1726	Comparison of density functionals for energy and structural differences between the high- $[\text{5T}2\text{g}: \text{t}2\text{g}]^4(\text{eg})^2$ and low- $[\text{1A}1\text{g}: \text{t}2\text{g}]^6(\text{eg})^0$ spin states of the hexaquoferrous cation $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$. <i>Journal of Chemical Physics</i> , 2004, 120, 9473-9486.	1.2	174
1727	Self-Exchange Electron Transfer Kinetics and Reduction Potentials for Anthraquinone Disulfonate. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3292-3303.	1.1	46
1728	DFT:B3LYPab initiomolecular dynamics study of the Zundel and Eigen proton complexes, H_5O_2^+ and H_9O_4^+ , in the triplet state in gas phase and solution. <i>Journal of Chemical Physics</i> , 2004, 120, 1217-1222.	1.2	15
1729	Theoretical Study of the Spin Trapping of Hydroxyl Radical by Cyclic Nitrones: A Density Functional Theory Approach. <i>Journal of the American Chemical Society</i> , 2004, 126, 1816-1829.	6.6	52
1730	Double hydrogen tunneling revisited: The breakdown of experimental tunneling criteria. <i>Journal of Chemical Physics</i> , 2004, 120, 11650-11657.	1.2	54

#	ARTICLE	IF	CITATIONS
1731	Broken-symmetry unrestricted hybrid density functional calculations on nickel dimer and nickel hydride. <i>Journal of Chemical Physics</i> , 2004, 121, 10026-10040.	1.2	19
1732	Solvothermal Syntheses, Crystal Structures, and Thermal Properties of New Manganese Thioantimonates(III): The First Example of the Thermal Transformation of an Amine-Rich Thioantimonate into an Amine-Poorer Thioantimonate. <i>Inorganic Chemistry</i> , 2004, 43, 2914-2921.	1.9	84
1733	Theoretical Investigation of the 3,4-Ethylenedioxythiophene Dimer and Unsubstituted Heterocyclic Derivatives. <i>Journal of Physical Chemistry A</i> , 2004, 108, 1440-1447.	1.1	48
1734	Strong Electronic Coupling between Dimolybdenum Units Linked by the N,N-Dimethyloxamidate Anion in a Molecule Having a Heteronaphthalene-like Structure. <i>Journal of the American Chemical Society</i> , 2004, 126, 14822-14831.	6.6	46
1735	Dissociative Adsorption of Methylsilane on the Si(100)-2 × 1 Surface. <i>Journal of Physical Chemistry B</i> , 2004, 108, 15103-15109.	1.2	12
1736	Computational Modeling of η^5 -Zirconocene Amide Complexes. <i>Organometallics</i> , 2004, 23, 5671-5680.	1.1	8
1737	Basic Density-Functional Theory an Overview. <i>Physica Scripta</i> , 2004, T109, 9.	1.2	87
1738	Photoelectron Spectroscopy of Free Polyoxoanions Mo ₆ O ₁₉ ²⁻ and W ₆ O ₁₉ ²⁻ in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10089-10093.	1.1	54
1739	Gallium Clusters Ga _n (n = 1-6): Structures, Thermochemistry, and Electron Affinities. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7448-7459.	1.1	41
1740	Electron Attachment to the Gas-Phase DNA Bases Cytosine and Thymine. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6562-6569.	1.1	191
1741	Steric Retardation of S _N 2 Reactions in the Gas Phase and Solution. <i>Journal of the American Chemical Society</i> , 2004, 126, 9054-9058.	6.6	174
1742	C-C Bond Cleavage of Acetonitrile by a Carbonyl Iron Complex with a Silyl Ligand. <i>Organometallics</i> , 2004, 23, 117-126.	1.1	120
1743	A multimode analysis of the gas-phase photoelectron spectra in oligoacenes. <i>Journal of Chemical Physics</i> , 2004, 120, 7490-7496.	1.2	163
1744	Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Study of the Deacylation Reaction in a Penicillin Binding Protein (PBP) versus in a Class C β -Lactamase. <i>Journal of the American Chemical Society</i> , 2004, 126, 7652-7664.	6.6	77
1745	Prediction of Two-Photon Absorption Properties for Organic Chromophores Using Time-Dependent Density-Functional Theory. <i>Journal of Physical Chemistry B</i> , 2004, 108, 899-907.	1.2	178
1746	Oxygen isotope exchange kinetics between H ₂ O and H ₄ SiO ₄ from ab initio calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2004, 68, 949-958.	1.6	13
1747	Important roles of tyrosines in Photosystem II and cytochrome oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2004, 1655, 45-50.	0.5	29
1748	Theoretical study of the polymer molecules (TeO ₂) _n as model systems for the local structure in TeO ₂ glass. <i>Journal of Non-Crystalline Solids</i> , 2004, 345-346, 734-737.	1.5	26

#	ARTICLE	IF	CITATIONS
1749	Dioxygen Activation at a Single Copper Site: Structure, Bonding, and Mechanism of Formation of 1:1 Cu ⁺ O ₂ Adducts. <i>Journal of the American Chemical Society</i> , 2004, 126, 16896-16911.	6.6	184
1750	The Performance of Hybrid Density Functionals in Solid State Chemistry. <i>Structure and Bonding</i> , 2004, , 171-232.	1.0	171
1751	DFT Computation of Relative Spin-State Energetics of Transition Metal Compounds. <i>Structure and Bonding</i> , 2004, , 151-184.	1.0	224
1752	Calculation of indirect nuclear spin-spin coupling constants within the regular approximation for relativistic effects. <i>Journal of Chemical Physics</i> , 2004, 120, 11407-11422.	1.2	60
1753	Combined Spectroscopic and Theoretical Study of Narrow Band Gap Heterocyclic Co-oligomers Containing Alternating Aromatic Donor and Quinoid Acceptor Units. <i>Journal of Physical Chemistry B</i> , 2004, 108, 2516-2526.	1.2	66
1754	Origins of Enantioselectivity in Reductions of Ketones on Cinchona Alkaloid Modified Platinum. <i>Journal of the American Chemical Society</i> , 2004, 126, 199-203.	6.6	99
1755	Spectroscopic Properties and Quantum Chemistry-Based Normal Coordinate Analysis (QCB-NCA) of a Dinuclear Tantalum Complex Exhibiting the Novel Side-On End-On Bridging Geometry of N ₂ : Correlations to Electronic Structure and Reactivity. <i>Journal of the American Chemical Society</i> , 2004, 126, 280-290.	6.6	47
1756	Synthesis, Biological Activity, and Three-Dimensional Quantitative Structure-Activity Relationship Model for a Series of Benzo[c]quinolizin-3-ones, Nonsteroidal Inhibitors of Human Steroid 5 α -Reductase 1. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 3546-3560.	2.9	28
1757	The Vibronic Structure of Electronic Absorption Spectra of Large Molecules: A Time-Dependent Density Functional Study on the Influence of Exact-Hartree-Fock Exchange. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10225-10237.	1.1	319
1758	Efficient hybrid density functional calculations in solids: Assessment of the Heyd-Scuseria-Ernzerhof screened Coulomb hybrid functional. <i>Journal of Chemical Physics</i> , 2004, 121, 1187-1192.	1.2	1,932
1759	Quantitative Structure-Activity Relationship for Cyclic Imide Derivatives of Protoporphyrinogen Oxidase Inhibitors: A Study of Quantum Chemical Descriptors from Density Functional Theory. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 2099-2105.	2.8	66
1760	Electronic and magnetic structure of LaMnO ₃ from hybrid periodic density-functional theory. <i>Physical Review B</i> , 2004, 69, .	1.1	116
1761	Binding of Benzylpenicillin to Metallo-lactamase: A QM/MM Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 17639-17648.	1.2	25
1762	Development and Assessment of a New Hybrid Density Functional Model for Thermochemical Kinetics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2715-2719.	1.1	639
1763	Developing Active Site Models of ODCase from Large Quantum Models to a QM/MM Approach. <i>Topics in Current Chemistry</i> , 2004, , 79-112.	4.0	7
1764	Electron-Rich Radicals by Neutralization-Reionization Mass Spectrometry. Generation, Dissociations and Energetics of the Hydrogen Atom Adduct to Acetamide. <i>European Journal of Mass Spectrometry</i> , 2004, 10, 869-879.	0.5	7
1765	Ring Complexes of S-Nitrosothiols with Cu ⁺ : A Density Functional Theory Study. <i>European Journal of Mass Spectrometry</i> , 2004, 10, 941-948.	0.5	4
1766	Li ⁺ vs Cu ⁺ Association to Toluene, Phenylsilane and Phenylgermane. Conventional vs Non-Conventional π -Complexes. <i>European Journal of Mass Spectrometry</i> , 2004, 10, 921-929.	0.5	8

#	ARTICLE	IF	CITATIONS
1767	A theoretical study of structural factors correlated with ^{23}Na NMR parameters. <i>American Mineralogist</i> , 2004, 89, 1314-1322.	0.9	9
1768	DFT Method Estimation of Standard Redox Potential of Metals. <i>Chemistry Letters</i> , 2004, 33, 1176-1177.	0.7	4
1769	Periodic solids and electron bands. , 2004, , 73-99.		1
1770	The Kohn-Sham auxiliary system. , 2004, , 135-151.		1
1771	Functionals for exchange and correlation. , 2004, , 152-171.		3
1772	Plane waves and grids: basics. , 2004, , 236-253.		0
1773	Localized orbitals: tight-binding. , 2004, , 272-297.		0
1774	Localized orbitals: full calculations. , 2004, , 298-312.		0
1775	Augmented functions: APW, KKR, MTO. , 2004, , 313-344.		0
1776	Quantum molecular dynamics (QMD). , 2004, , 371-386.		0
1777	Excitation spectra and optical properties. , 2004, , 406-417.		0
1783	Augmented functions: linear methods. , 2004, , 345-368.		0
1786	Density functional theory: foundations. , 2004, , 119-134.		6
1787	Comparative Structural Studies of 4-Diazopyrazole Derivatives by X-Ray Diffraction and Theoretical Investigation. <i>Heterocycles</i> , 2005, 65, 2753.	0.4	5
1788	Relationships between Light-Emitting Properties and Different Isomers in Polymorphs of Tris(8-hydroxyquinoline) Aluminum(III) (Alq_3) Analyzed by Solid-State ^{27}Al NMR and Density Functional Theory (DFT) Calculations. <i>Japanese Journal of Applied Physics</i> , 2005, 44, 3706-3711.	0.8	31
1789	The Structural and Electronic Properties of C_{16} Benzene onto Cu_5 (100) Cluster Using ab initio Molecular Orbital Method. <i>Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals</i> , 2005, 69, 121-126.	0.2	0
1790	Radicals Derived from Guanine: Structures and Energetics. <i>Collection of Czechoslovak Chemical Communications</i> , 2005, 70, 826-836.	1.0	19
1791	Theoretical Study on Acylacetanilide Azomethine Dyes: A Relationship between Electronic Absorption Properties and Molecular Structures. <i>Bulletin of the Chemical Society of Japan</i> , 2005, 78, 1929-1938.	2.0	4

#	ARTICLE	IF	CITATIONS
1792	Determination of the absolute configuration of chiral α -aryloxypropanoic acids using vibrational circular dichroism studies: 2-(2-chlorophenoxy) propanoic acid and 2-(3-chlorophenoxy) propanoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 61, 1327-1334.	2.0	12
1793	FTIR, FT-Raman spectra and ab initio DFT vibrational analysis of 2-bromo-4-methyl-phenylamine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 62, 740-751.	2.0	101
1794	Aggregation of acetic and propionic acid in argon matrices—A matrix isolation and computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 62, 902-909.	2.0	52
1795	Titanium-catalyzed iminohydrazination of alkynes. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 5066-5077.	0.8	69
1796	Synthesis and quadratic molecular hyperpolarizabilities of two new chiral boronates: Computational and experimental study. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 3737-3745.	0.8	13
1797	Development of 7-membered N-heterocyclic carbene ligands for transition metals. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 6143-6155.	0.8	86
1798	Origin and features of the electrochemiluminescence of luminol — Experimental and theoretical investigations. <i>Journal of Electroanalytical Chemistry</i> , 2005, 580, 41-49.	1.9	29
1799	An extremely stable Ni(II) complex derived from the hydrolytic cleavage of the C-terminal tail of histone H2A. <i>Journal of Inorganic Biochemistry</i> , 2005, 99, 637-643.	1.5	16
1800	Vibrational dynamics study of the effect of the substituents on the π -conjugation of different bithiophene molecules. <i>Journal of Molecular Structure</i> , 2005, 744-747, 393-401.	1.8	4
1801	FT-Raman spectroscopic study, aided by quantum chemical DFT calculations, of a series of oligothiophenes end-capped by nitriles. <i>Journal of Molecular Structure</i> , 2005, 744-747, 403-409.	1.8	6
1802	Combined theoretical and spectroscopic Raman study of 3,4-ethylenedioxy and S,S-dioxide substituted terthiophenes and their parent polymers. <i>Journal of Molecular Structure</i> , 2005, 744-747, 551-556.	1.8	5
1803	Molecular properties of the product radical in adenosylcobalamin-dependent ethanolamine deaminase. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2005, 350, 131-143.	1.2	1
1804	Toward a general mechanism of electron capture dissociation. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 208-224.	1.2	308
1805	A comparison of the gas phase acidities of phospholipid headgroups: Experimental and computational studies. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 926-939.	1.2	45
1806	Experimental and theoretical investigations of the loss of amino acid side chains in electron capture dissociation of model peptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 1523-1535.	1.2	89
1807	Protonated adenine: Tautomers, solvated clusters, and dissociation mechanisms. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 1713-1726.	1.2	69
1808	Simple b ions have cyclic oxazolone structures. A neutralization-reionization mass spectrometric and computational study of oxazolone radicals. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 1941-1956.	1.2	28
1809	Structural and electronic effects induced by carboxylic acid substitution in isomeric 2,2'-bithiophenes and oligothiophenes: A computational study. <i>Polymer</i> , 2005, 46, 9452-9460.	1.8	29

#	ARTICLE	IF	CITATIONS
1810	Reaction pathways for Zn(II)-catalyzed carboxylic acid esters hydrolysis. <i>Inorganica Chimica Acta</i> , 2005, 358, 77-92.	1.2	8
1811	Experimental and DFT studies on the DNA-binding trend and spectral properties of complexes [Ru(bpy)2L]2+ (L=dmdpq, dpq, and dcdpq). <i>Inorganica Chimica Acta</i> , 2005, 358, 3311-3319.	1.2	75
1812	Synthesis, characterization, structures and DNA-binding properties of complexes [Ru(bpy)2(L)]2+ (L=ptdb, ptda and ptdp) with asymmetric intercalative ligands. <i>Inorganica Chimica Acta</i> , 2005, 358, 3430-3440.	1.2	47
1813	Theoretical methods that help understanding the structure and reactivity of gas phase ions. <i>International Journal of Mass Spectrometry</i> , 2005, 240, 37-99.	0.7	104
1814	The aluminum phosphides AlmPn (m+n=2â€“5) and their anions: structures, electron affinities and vibrational frequencies. <i>International Journal of Mass Spectrometry</i> , 2005, 240, 149-159.	0.7	15
1815	The alkylethynyl radicals, CCCnH2n+1 (n=1âˆ“4), and their anions. <i>International Journal of Mass Spectrometry</i> , 2005, 241, 295-304.	0.7	20
1816	Mechanism of nitrogen-enhanced negative bias temperature instability in pMOSFET. <i>Microelectronics Reliability</i> , 2005, 45, 19-30.	0.9	34
1817	Geometric and electronic structure of the diphenylamine radical cation: an EPR, ENDOR and MO study. <i>Journal of Molecular Structure</i> , 2005, 733, 13-17.	1.8	8
1818	Conformational and NBO analysis on cis and trans isomers of methyl-1-(4-hydroxy-3-methoxyphenyl)-1,2,3,4-tetrahydro-9H-âˆ“2-carboline-3-carboxylate. <i>Journal of Molecular Structure</i> , 2005, 754, 45-50.	1.8	3
1819	Synthesis, characterization and computational modeling of cyclen substituted with dendrimeric branches. Dendrimeric and macrocyclic moieties working together in a collective fashion. <i>Journal of Molecular Structure</i> , 2005, 779, 1-10.	1.8	8
1820	Structureâ€“activity relationships for inhibition of human cholinesterases by alkyl amide phenothiazine derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 211-222.	1.4	55
1821	Amentoflavone and its derivatives as novel natural inhibitors of human Cathepsin B. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 5819-5825.	1.4	57
1822	Why does the hydrolysis of In(III) aquacomplexes make them electrochemically more active?. <i>Electrochimica Acta</i> , 2005, 50, 4888-4896.	2.6	20
1823	Influence of (S)-1-phenylethylamine para substitution on the resolution of (Â±)-1,4-benzodioxane-2-carboxylic acid: a crystallographic, theoretical and morphologic approach. <i>Tetrahedron: Asymmetry</i> , 2005, 16, 2099-2106.	1.8	16
1824	Density functional complete study of hydrogen bonding between the dichlorine monoxide and the hydroxyl radical (Cl2Oâˆ“HO). <i>Computational and Theoretical Chemistry</i> , 2005, 714, 7-12.	1.5	7
1825	Computational study on the addition of HCN to methanimine catalyzed by formamidine and formamide. <i>Computational and Theoretical Chemistry</i> , 2005, 713, 51-57.	1.5	4
1826	Effects of conjugation length and donorâ€“acceptor functionalization on the non-linear optical properties of organic pushâ€“pull molecules using density functional theory. <i>Computational and Theoretical Chemistry</i> , 2005, 715, 59-64.	1.5	27
1827	Hydrogen abstraction from dimethyl ether (DME) and dimethyl sulfide (DMS) by OH radical: a computational study. <i>Computational and Theoretical Chemistry</i> , 2005, 722, 9-19.	1.5	43

#	ARTICLE	IF	CITATIONS
1828	Ab initio and DFT gas phase investigations of the C ₇ H ₁₁ ⁺ potential energy surfaces of bicyclobutonium species and related carbocations. Computational and Theoretical Chemistry, 2005, 718, 93-104.	1.5	7
1829	The small silicon clusters Si _n (n=2-10) and their anions: structures, thermochemistry, and electron affinities. Computational and Theoretical Chemistry, 2005, 719, 89-102.	1.5	85
1830	Carbon-hydrogen bond dissociation enthalpies in ethers: a theoretical study. Computational and Theoretical Chemistry, 2005, 719, 109-114.	1.5	25
1831	Theoretical study of the reactivity of X(3P) (X=Ge, Sn, Pb) with N ₂ O(X ¹ Σ ⁺). Computational and Theoretical Chemistry, 2005, 724, 185-193.	1.5	9
1832	Theoretical studies on the reaction OH+CH ₃ SiH ₂ CH ₃ . Computational and Theoretical Chemistry, 2005, 728, 25-29.	1.5	18
1833	Electronic structures and SARs of the isomeric complexes $\hat{1}^{\pm}$, $\hat{1}^2$, $\hat{1}^3$ - [Ru(mazpy) ₂ Cl ₂] with different antitumor activities. Computational and Theoretical Chemistry, 2005, 728, 93-101.	1.5	16
1834	A theoretical study on Cu(II)-chelating properties of curcumin and its implications for curcumin as a multipotent agent to combat Alzheimer's disease. Computational and Theoretical Chemistry, 2005, 757, 199-202.	1.5	43
1835	A Theoretical Study on the Potential Energy Surface of the 1C ₃ + NO Reaction. Computational and Theoretical Chemistry, 2005, 730, 207-215.	1.5	7
1836	Theoretical study on the aromaticity of the bimetallic clusters X ₂ M ₂ (X=Si, Ge, M=Al, Ga). Computational and Theoretical Chemistry, 2005, 732, 149-153.	1.5	17
1837	DFT study on the electron affinities of the chlorinated benzenes. Computational and Theoretical Chemistry, 2005, 732, 63-70.	1.5	9
1838	Structures and electron affinities of silicon hydrides Si ₄ H _n (n=2-10). Computational and Theoretical Chemistry, 2005, 755, 65-74.	1.5	11
1839	Low-lying energy levels of amino acids and its implications for origin of life. Computational and Theoretical Chemistry, 2005, 756, 109-112.	1.5	8
1840	A QSAR study of substituted benzo[a]phenazines as potential anticancer agents. Computational and Theoretical Chemistry, 2005, 756, 167-172.	1.5	19
1841	Solid state NMR and DFT study of polymer electrolyte poly(ethylene oxide)/LiCFSO. Solid State Ionics, 2005, 176, 163-167.	1.3	19
1842	Adsorption of halide ions from aqueous solutions at a Cd(0001) electrode surface: quantum chemical modelling and experimental study. Surface Science, 2005, 577, 112-126.	0.8	17
1843	Quinoxalines XIV. Synthesis, ¹ H, ¹³ C, ¹⁵ N NMR spectroscopic, and quantum chemical study of 1H-pyrazolo[3,4-b]quinoxalines (flavazoles). Tetrahedron, 2005, 61, 2373-2385.	1.0	5
1844	Application of ¹ J(C,H) coupling constants in conformational analysis. Tetrahedron, 2005, 61, 7349-7358.	1.0	36
1845	Radical hydrogen abstraction-cyclization with a 2-bromovinylsilyl group as a bifunctional tether. Tetrahedron, 2005, 61, 7865-7873.	1.0	5

#	ARTICLE	IF	CITATIONS
1846	A quantum chemical study on the mechanism of glycinamide ribonucleotide transformylase inhibitor: 10-Formyl-5,8,10-trideazafolic acid. <i>Biophysical Chemistry</i> , 2005, 118, 78-83.	1.5	0
1847	A new insight in the unusual adsorption properties of Cu ⁺ cations in Cu-ZSM-5 zeolite. <i>Catalysis Today</i> , 2005, 110, 281-293.	2.2	41
1848	Efficient generation of matrix elements for one-electron spin-orbit operators. <i>Chemical Physics</i> , 2005, 311, 71-79.	0.9	87
1849	Microscopic modelling of the reduction of a Zn(II) aqua-complex on metal electrodes. <i>Chemical Physics</i> , 2005, 310, 257-268.	0.9	32
1850	Calculation of ¹⁹ F NMR chemical shifts in uranium complexes using density functional theory and pseudopotentials. <i>Chemical Physics</i> , 2005, 311, 45-56.	0.9	37
1851	A combined theoretical and experimental investigation about the influence of the dopant in the anionic electropolymerization of 1,4-tetrathiothiophene. <i>Chemical Physics</i> , 2005, 314, 1-7.	0.9	12
1852	A DFT study on the deprotonation antioxidant mechanistic step of ortho-substituted phenolic cation radicals. <i>Chemical Physics</i> , 2005, 316, 195-204.	0.9	54
1853	Quickstep: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach. <i>Computer Physics Communications</i> , 2005, 167, 103-128.	3.0	4,200
1854	A joint theoretical and experimental study of phenylene-acetylene molecular wires. <i>Chemical Physics Letters</i> , 2005, 401, 149-156.	1.2	68
1855	Calculation of the enthalpies of formation for transition metal complexes. <i>Chemical Physics Letters</i> , 2005, 401, 58-61.	1.2	48
1856	A combined experimental and theoretical study of the conformation of N,N'-diphenyl-N,N'-di(m-tolyl)benzidine using solid-state ¹⁵ N NMR and DFT calculations. <i>Chemical Physics Letters</i> , 2005, 401, 246-253.	1.2	19
1857	Raman, infrared, SERS and DFT calculations of a triazole derivative (akacid). <i>Chemical Physics Letters</i> , 2005, 402, 361-366.	1.2	28
1858	Electronic properties of rhenium, osmium and iridium dimers by density functional methods. <i>Chemical Physics Letters</i> , 2005, 403, 367-371.	1.2	21
1859	Hydrogen bond stabilization in Diels-Alder transition states: The cycloaddition of hydroxy-ortho-quinodimethane with fumaric acid and dimethylfumarate. <i>Chemical Physics Letters</i> , 2005, 406, 355-359.	1.2	3
1860	A theoretical study on the strength of two-center three-electron bond in (CH ₃) ₂ S=OH and H ₂ S=OH adducts. <i>Chemical Physics Letters</i> , 2005, 408, 216-220.	1.2	14
1861	Dual-level direct dynamics studies on the reactions of OH radicals with SiH ₃ CH ₃ and SiH ₄ . <i>Chemical Physics Letters</i> , 2005, 409, 355-361.	1.2	3
1862	The torsional potential in 2,2'-bipyrrrole revisited: High-level ab initio and DFT results. <i>Chemical Physics Letters</i> , 2005, 411, 321-326.	1.2	15
1863	Selective functionalization of the Si(100) surface by a bifunctional alkynilamine molecule: A density functional study of the switching adsorption linkage. <i>Chemical Physics Letters</i> , 2005, 413, 473-478.	1.2	3

#	ARTICLE	IF	CITATIONS
1864	Does the Co ⁺ -assisted decarbonylation of acetaldehyde occur via C=C or C-H activation? A theoretical investigation using density functional theory. <i>Chemical Physics Letters</i> , 2005, 414, 28-33.	1.2	34
1865	Hybrid functional with separated range. <i>Chemical Physics Letters</i> , 2005, 415, 100-105.	1.2	243
1866	A theoretical study of the different radical-scavenging activities of catechin, quercetin, and a rationally designed planar catechin. <i>Bioorganic Chemistry</i> , 2005, 33, 108-115.	2.0	46
1867	A new multivalent cluster: synthesis, electrochemistry, solid state structure and computational studies on the iron-nickel mixed-metal nitride anions [Fe ₆ Ni ₆ N ₂ (CO) ₂₄] ⁿ⁻ (n=2-4). <i>Comptes Rendus Chimie</i> , 2005, 8, 1850-1855.	0.2	11
1868	Desulfurization of transportation fuels by π -complexation sorbents: Cu(I)-, Ni(II)-, and Zn(II)-zeolites. <i>Applied Catalysis B: Environmental</i> , 2005, 56, 111-126.	10.8	339
1869	Benchmark Databases for Nonbonded Interactions and Their Use To Test Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 415-432.	2.3	832
1870	Lipophilicity and Metabolic Route Prediction of Imidazolium Ionic Liquids * (6 pp). <i>Environmental Science and Pollution Research</i> , 2005, 12, 199-204.	2.7	62
1871	Copper(I)-Catalyzed Synthesis of Azoles. DFT Study Predicts Unprecedented Reactivity and Intermediates. <i>Journal of the American Chemical Society</i> , 2005, 127, 210-216.	6.6	1,497
1872	Theoretical Studies about the Influence of Different Ring Substituents on the Nucleophilic Ring Opening of Three-Membered Heterocycles and Possible Implications for the Mechanisms of Cysteine Protease Inhibitors. <i>Journal of Organic Chemistry</i> , 2005, 70, 233-237.	1.7	57
1873	Multidisciplinary Physicochemical Analysis of Oligothiophenes End-Capped by Nitriles: Δ Electrochemistry, UV-Vis-Near-IR, IR, and Raman Spectroscopies and Quantum Chemistry. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10115-10125.	1.2	40
1874	Cracking Electron Correlation. <i>Physica Scripta</i> , 2005, T120, 78-82.	1.2	6
1875	Formation of Ring-Like Si-O-Zr Bonds at Intergranular Interfaces in Silica-Doped Zirconia. <i>Journal of the American Ceramic Society</i> , 2005, 88, 1041-1045.	1.9	17
1876	Enantioselective hydrogenation of ethyl pyruvate catalyzed by - and -isocinchonine-modified Pt/AlO in toluene: inversion of enantioselectivity. <i>Journal of Catalysis</i> , 2005, 231, 33-40.	3.1	43
1877	Evaluation of a new copper(II)-curcumin complex as superoxide dismutase mimic and its free radical reactions. <i>Free Radical Biology and Medicine</i> , 2005, 39, 811-822.	1.3	208
1878	Synthesis, crystal structure and properties of K ₄ Ba ₂ (Nb ₂ S ₁₁) ₂ . <i>Solid State Sciences</i> , 2005, 7, 1062-1069.	1.5	7
1879	Electronic structure study of the initiation routes of the dimethyl sulfide oxidation by OH. <i>Journal of Computational Chemistry</i> , 2005, 26, 569-583.	1.5	27
1880	Agreement between experiment and hybrid DFT calculations for O-H bond dissociation enthalpies in manganese complexes. <i>Journal of Computational Chemistry</i> , 2005, 26, 661-667.	1.5	39
1881	Importance of accurate charges in molecular docking: Quantum mechanical/molecular mechanical (QM/MM) approach. <i>Journal of Computational Chemistry</i> , 2005, 26, 915-931.	1.5	365

#	ARTICLE	IF	CITATIONS
1882	Quantum chemical modeling of CO oxidation by the active site of molybdenum CO dehydrogenase. <i>Journal of Computational Chemistry</i> , 2005, 26, 888-898.	1.5	72
1883	Lennard-Jones parameters for the combined QM/MM method using the B3LYP/6-31G*/AMBER potential. <i>Journal of Computational Chemistry</i> , 2005, 26, 1270-1278.	1.5	82
1884	A joint study based on the electron localization function and catastrophe theory of the chameleonic and centauric models for the Cope rearrangement of 1,5-hexadiene and its cyano derivatives. <i>Journal of Computational Chemistry</i> , 2005, 26, 1427-1437.	1.5	56
1885	Benchmarking approximate density functional theory. I.s/d excitation energies in 3d transition metal cations. <i>Journal of Computational Chemistry</i> , 2005, 26, 1505-1518.	1.5	57
1886	Dual-level direct dynamics studies on the reaction Cl + CHBr ₂ Cl. <i>Journal of Computational Chemistry</i> , 2005, 26, 1421-1426.	1.5	2
1887	Gold(0) and Gold(III) Reactivity towards the Tetraphenyldithioimidodiphosphinic Acid, [Ph ₂ P(S)NHP(S)Ph ₂]. <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 589-596.	1.0	16
1888	First-Row Transition Metal Bis(amidinate) Complexes; Planar Four-Coordination of FeII Enforced by Sterically Demanding Aryl Substituents. <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 2089-2099.	1.0	66
1889	Photoelectron Spectra and Electronic Structures of Substituted Pyrimidines. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 522-531.	1.2	16
1890	Reactive Et ₃ C(p-p)I ⁻ -systems 53 [1]: Reactivity studies on perfluoro-2-arsapropene: [2+2]-cycloaddition reactions and quantum chemical calculations. <i>Heteroatom Chemistry</i> , 2005, 16, 406-419.	0.4	5
1891	Activation Energies and Reaction Energetics for 1,3-Dipolar Cycloadditions of Hydrazoic Acid with C≡C and C≡N Multiple Bonds from High-Accuracy and Density Functional Quantum Mechanical Calculations. <i>Helvetica Chimica Acta</i> , 2005, 88, 1702-1710.	1.0	28
1892	Through versus Cross Electron Delocalization in Polytriacetylene Oligomers: A Computational Analysis. <i>ChemPhysChem</i> , 2005, 6, 511-519.	1.0	16
1893	Ab Initio Molecular Dynamics Simulation of a Water-Hydrogen Fluoride Equimolar Mixture. <i>ChemPhysChem</i> , 2005, 6, 148-153.	1.0	20
1894	A Theoretical Study on the Low-Lying Excited States of 2,2,5,5-Terthiophene and 2,2,5,5-Quaterthiophene. <i>ChemPhysChem</i> , 2005, 6, 1357-1368.	1.0	37
1895	Assessment of Density Functionals for the High-Spin/Low-Spin Energy Difference in the Low-Spin Iron(II) Tris(2,2'-bipyridine) Complex. <i>ChemPhysChem</i> , 2005, 6, 1393-1410.	1.0	162
1896	Kinetic and DFT Studies on the Ag/TiO ₂ -Photocatalyzed Selective Reduction of Nitrobenzene to Aniline. <i>ChemPhysChem</i> , 2005, 6, 1537-1543.	1.0	64
1897	Kinetic and DFT Studies on the Photoinduced Desorption of Sulfur from Gold Nanoparticles Loaded on Titanium Dioxide. <i>ChemPhysChem</i> , 2005, 6, 2508-2512.	1.0	8
1898	Proton Sandwiches: Nonclassical Carbocations with Tetracoordinate Protons. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2719-2723.	7.2	45
1899	Derivatives of the Simplest Polyhedral Carborane Anion: Structures at the Borderline between Two- and Three-Dimensional Aromatic Compounds. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 1643-1646.	7.2	19

#	ARTICLE	IF	CITATIONS
1900	Polyhedral Vanadium Oxide Cages: Infrared Spectra of Cluster Anions and Size-Induced d Electron Localization. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 3122-3125.	7.2	116
1901	Dimethyl Carbonate in the Supercages of NaY Zeolite: The Role of Local Fields in Promoting Methylation and Carboxymethylation Activity. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 4774-4777.	7.2	48
1902	Intramolecular Rotation through Proton Transfer: $[\text{Fe}(\eta^5\text{-C}_5\text{H}_4\text{CO}_2^-)_2]$ versus $[(\eta^5\text{-C}_5\text{H}_4\text{CO}_2^-)\text{Fe}(\eta^5\text{-C}_5\text{H}_4\text{CO}_2\text{H})]$. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 6022-6024.	7.2	41
1903	Observation of d-Orbital Aromaticity. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 7251-7254.	7.2	197
1910	The Direct, Enantioselective, One-Pot, Three-Component, Cross-Mannich Reaction of Aldehydes: The Reason for the Higher Reactivity of Aldimine versus Aldehyde in Proline-Mediated Mannich and Aldol Reactions. <i>Advanced Synthesis and Catalysis</i> , 2005, 347, 1595-1604.	2.1	44
1911	Spectroscopic characterization of the conformational states of the bis(trifluoromethanesulfonyl)imide anion (TFSI ⁻). <i>Journal of Raman Spectroscopy</i> , 2005, 36, 762-770.	1.2	321
1912	Selenoketene ($\text{H}_2\text{C}=\text{C}=\text{C}=\text{Se}$) and selenoketyl cumulene ($\text{HC}=\text{C}=\text{C}=\text{Se}$) ions and their neutral counterparts: a tandem mass spectrometric and computational study. <i>Journal of Mass Spectrometry</i> , 2005, 40, 796-806.	0.7	5
1913	Gas-phase tautomers of protonated 1-methylcytosine. Preparation, energetics, and dissociation mechanisms. <i>Journal of Mass Spectrometry</i> , 2005, 40, 1417-1428.	0.7	25
1914	Absolute configurations of chiral herbicides determined from vibrational circular dichroism. <i>Chirality</i> , 2005, 17, S1-S8.	1.3	19
1915	Lewis Adducts of the Side-On End-On Dinitrogen-Bridged Complex $[\{(\text{NPN})\text{Ta}\}_2(\eta^2\text{-H})_2(\eta^1\text{-N}_2)]$ with AlMe_3 , GaMe_3 , and $\text{B}(\text{C}_6\text{F}_5)_3$: Synthesis, Structure, and Spectroscopic Properties. <i>Chemistry - A European Journal</i> , 2005, 11, 604-618.	1.7	42
1916	Xenophilic Complexes Bearing a TpR Ligand, $[\text{TpRM}^n\text{M}^n\text{Ln}]$ [$\text{TpR}=\text{Tp}^i\text{Pr}_2$, $\text{Tp}^\#$ ($\text{TpMe}_{2,4}\text{-Br}$); $\text{M}=\text{Ni}$, Co , Fe , Mn ; $\text{M}^n\text{Ln}=\text{Co}(\text{CO})_4$, $\text{Co}(\text{CO})_3(\text{PPh}_3)$, $\text{RuCp}(\text{CO})_2$]: The Two Metal Centers are Held Together not by Covalent Interaction but by Electrostatic Attraction. <i>Chemistry - A European Journal</i> , 2005, 11, 2788-2809.	1.7	25
1917	Computational Study of Structures and Properties of Metallaboranes: Cobalt Bis(dicarbollide). <i>Chemistry - A European Journal</i> , 2005, 11, 4109-4120.	1.7	65
1918	Nonlinear Optical Properties in Calix[n]arenes: Orientation Effects of Monomers. <i>Chemistry - A European Journal</i> , 2005, 11, 4961-4969.	1.7	35
1919	Triple-Bond Covalent Radii. <i>Chemistry - A European Journal</i> , 2005, 11, 3511-3520.	1.7	370
1920	Heavy Group 14 1,(n+2)-Dimetallabicyclo[n.n.n]alkanes and 1,(n+2)-Dimetalla[n.n.n]propellanes: Are They All Realistic Synthetic Targets?. <i>Chemistry - A European Journal</i> , 2005, 11, 5067-5079.	1.7	27
1921	Geometric and electronic similarities between transition structures for electrocyclizations and sigmatropic hydrogen shifts. <i>Theoretical Chemistry Accounts</i> , 2005, 113, 205-211.	0.5	6
1922	Structure-activity study of thiazides by magnetic resonance methods (NQR, NMR, EPR) and DFT calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2005, 23, 329-337.	1.3	17
1923	Olefin hydrogenation using diimine pyridine complexes of Co and Rh. <i>Journal of Molecular Catalysis A</i> , 2005, 232, 151-159.	4.8	129

#	ARTICLE	IF	CITATIONS
1924	A combined experimental and molecular modeling approach for ethene-propene copolymerization with C2-symmetric metallocenes. <i>Journal of Molecular Catalysis A</i> , 2005, 242, 91-104.	4.8	21
1925	Pathways for proton migration over the surface of a metal-cyclotriphosphorus cluster. <i>Comptes Rendus Chimie</i> , 2005, 8, 1535-1542.	0.2	1
1926	Ion/molecule reactions of 2-chloro- and 2-bromopropene radical cations with methanol and ethanol FT-ICR spectrometry and DFT calculations. <i>International Journal of Mass Spectrometry</i> , 2005, 241, 31-42.	0.7	5
1927	Theoretical investigations on CH ₂ CH=CH ₂ OH on the Si(100)-2 \times 1 and Ge(100)-2 \times 1 surfaces. <i>Surface Science</i> , 2005, 586, 45-55.	0.8	16
1928	Density functional theory study of initial stage of ZrO ₂ atomic layer deposition on Ge/Si(100)-(2 \times 1) surface. <i>Thin Solid Films</i> , 2005, 479, 73-76.	0.8	5
1929	Binding of transition metal complexes to guanine and guanine-cytosine: hydrogen bonding and covalent effects. <i>Journal of Biological Inorganic Chemistry</i> , 2005, 10, 854-866.	1.1	37
1930	Hydrogen-bond effects on the electronic absorption spectrum and evaluation of nonlinear optical properties of an aminobenzodifuranone derivative that exhibits the largest positive solvatochromism. <i>Journal of Molecular Modeling</i> , 2005, 11, 317-322.	0.8	16
1931	Reinvestigation of molecular structure and barrier to internal rotation of pyridinium N-phenolate betaine dye. <i>Journal of Molecular Modeling</i> , 2005, 11, 392-397.	0.8	3
1932	Synthesis, characterization and DNA-binding properties of mixed porphyrin-polypyridyl ruthenium(II) complexes. <i>Transition Metal Chemistry</i> , 2005, 30, 82-88.	0.7	20
1933	Ab initio calculation of nitrogen oxide dimer structure and its anion-radical. <i>Journal of Structural Chemistry</i> , 2005, 46, 213-219.	0.3	4
1934	MoS ₂ single slab as a model for active component of hydrodesulfuration catalyst: a quantum chemical study 1. Molecular and electronic structure of Mo ₁₂ S ₂₄ macromolecule and its adsorption complex with H ₂ S. <i>Russian Chemical Bulletin</i> , 2005, 54, 2259-2263.	0.4	3
1935	Reaktive E=C(p-p)-Systeme. 54 [1] Reaktionen des Perfluor-2-arsapropens, F ₃ CA _s =CF ₂ (1), mit H-aciden Verbindungen Me ₂ EH (E = N, P, As) und MeE $\hat{=}$ H (E $\hat{=}$ = O, S, Se). <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2005, 631, 1430-1438.	0.6	3
1936	Strong Electronic Coupling between Mo ₂ ⁿ⁺ Units: The Oxidation Products of [Mo ₂ (DAniF) ₃] ₂ ($\frac{1}{4}$ H) ₂ and Mo ₂ (DAniF) ₄ . <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2005, 631, 2606-2612.	0.6	26
1937	Geometries and electronic structures of W ₄ and W ₇ clusters. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 334-339.	1.0	1
1938	Ab initio and DFT investigation of the structures and properties of chloromethyl and chlorofluoromethyl peroxy radicals. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 178-188.	1.0	5
1939	Principal component analysis of the effects of wavefunction modification on the electrostatic potential of indole. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 379-386.	1.0	1
1940	Chemical reaction dynamics of PeCB and TCDD decomposition: A tight-binding quantum chemical molecular dynamics study with first-principles parameterization. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 318-327.	1.0	21
1941	Theoretical investigation of the mechanism of the intermolecular proton transfer in carbanion [1.1]ferrocenophane. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 847-857.	1.0	1

#	ARTICLE	IF	CITATIONS
1942	Density functional study of the heme moiety of cytochrome c. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 1002-1009.	1.0	8
1943	Localized hybrid exchange-correlation potentials for Kohn-Sham DFT calculations of NMR and EPR parameters. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 261-271.	1.0	30
1944	Spectroscopic and DFT studies of donor-acceptor molecules containing phenylquinoline and phenothiazine moieties in various redox states. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 635-644.	1.0	7
1945	Local HSAB principle in the conjugate addition of p-substituted thiophenols to cyclohexenone. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 29-37.	1.0	10
1946	Ab initio studies on the polarizability of lithium clusters: Some unusual results. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 166-173.	1.0	21
1947	Hydrogen bond character and proton transfer behavior in water-thiophenol clusters and their cation radicals: Insight into water number size dependence. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 186-198.	1.0	2
1948	Density functional theory study of the relative energies and structures of the chair, twist, and boat conformations of stannacyclohexane, 1-methylstannacyclohexane, and 1,1-dimethylstannacyclohexane. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 416-428.	1.0	5
1949	Chemical bonding, less screening, and Hund's rule revisited. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 687-700.	1.0	9
1950	Geometry and binding properties of different multiple-state glycine-Fe ⁺ /Fe ²⁺ complexes. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 26-34.	0.9	18
1951	NMR and DFT investigations of the substituent and solvent effect on amino-imino tautomerism in acridin-9-amines substituted at the exocyclic nitrogen atom. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 870-879.	0.9	12
1952	La modelizaci3n molecular como herramienta para el dise±o de nuevos pol3meros conductores. <i>Polimeros</i> , 2005, 15, 239-244.	0.2	3
1953	Structure of SnCl ₂ ·1-ethyl-3-methylimidazolium Chloride Ambient-Temperature Molten Salt using Density Functional Theory Calculation and Raman Spectroscopy. <i>Electrochemistry</i> , 2005, 73, 715-723.	0.6	3
1954	Applied density functional theory and the deMon codes 1964â€“2004. , 2005, , 1079-1097.		4
1955	Quantum chemical study of adsorption and dissociation of HfCl ₄ and H ₂ O on Ge/Si(100) $\hat{\sim}$ (2Å–1): Initial stage of atomic layer deposition of HfO ₂ on SiGe surface. <i>Journal of Materials Research</i> , 2005, 20, 586-591.	1.2	0
1956	Initial surface reactions in atomic layer deposition of Al ₂ O ₃ on the hydroxylated GaAs(001)-4 Å– 2 surface. <i>Journal of Physics Condensed Matter</i> , 2005, 17, 7517-7522.	0.7	9
1957	Study of Pathway of Hydrogen Migration and Desorption on SiGe(100) Surface Using Ab Initio Calculations. <i>Japanese Journal of Applied Physics</i> , 2005, 44, 7625-7633.	0.8	4
1958	Methods and models for studying mechanisms of redox-active enzymes. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2005, 363, 847-860.	1.6	21
1959	Orbital-dependent correlation energy in density-functional theory based on a second-order perturbation approach: Success and failure. <i>Journal of Chemical Physics</i> , 2005, 123, 062204.	1.2	99

#	ARTICLE	IF	CITATIONS
1960	Infrared-visible and visible-visible double resonance spectroscopy of 1-hydroxy-9,10-anthraquinone-(H ₂ O) π - π^* (n=1,2) complexes. Journal of Chemical Physics, 2005, 122, 034305.	1.2	8
1961	Accurate prediction for electron affinities of the radicals derived from the halide benzene. Journal of Chemical Physics, 2005, 123, 084320.	1.2	3
1962	Linear scaling computation of the Fock matrix. VIII. Periodic boundaries for exact exchange at the Γ point. Journal of Chemical Physics, 2005, 122, 124105.	1.2	24
1963	Initial-stage oxidation mechanism of Ge(100) 2×1 dimers. Physical Review B, 2005, 72, .	1.1	22
1964	Phosphine adsorption and dissociation on the Si(001) surface: An ab initio survey of structures. Physical Review B, 2005, 72, .	1.1	44
1965	Density functional theory study of adsorption and dissociation of HfCl ₄ and H ₂ O on Ge π -Si(100)-(2 \times 1): Initial stage of atomic layer deposition of HfO ₂ on SiGe surface. Applied Physics Letters, 2005, 86, 142901.	1.5	5
1966	Accurate molecular energies by extrapolation of atomic energies using an analytic quantum mechanical model. Physical Review B, 2005, 71, .	1.1	14
1967	Relativistic second-order many-body and density-functional theory for the parity-violation contribution to the C π -F stretching mode in CHFClBr. Physical Review A, 2005, 71, .	1.0	42
1968	First-principle computation of zero-field splittings: Application to a high valent Fe(IV)-oxo model of nonheme iron proteins. Journal of Chemical Physics, 2005, 123, 204902.	1.2	41
1969	Structure and formation mechanism of six-fold coordinated silicon in phosphosilicate glasses. Physical Review B, 2005, 71, .	1.1	38
1970	A combined crossed-beam and theoretical investigation of radical-radical reaction dynamics of O(P3)+t-C ₄ H ₉ $\hat{\pi}$ ⁺ OH+iso-C ₄ H ₈ . Journal of Chemical Physics, 2005, 123, 211105.	1.2	13
1971	An ab initio study of the vibronic, spin π -orbit, and magnetic hyperfine structure in the X $\hat{1}^2$ electronic state of NCO. Journal of Chemical Physics, 2005, 122, 144306.	1.2	8
1972	Comparison of density functionals for energy and structural differences between the high- [5T _{2g} :(t _{2g}) ⁴ (e _g) ²] and low- [1A _{1g} :(t _{2g}) ⁶ (e _g) ⁰] spin states of iron(II) coordination compounds. II. More functionals and the hexaminoferrous cation, [Fe(NH ₃) ₆] ²⁺ . Journal of Chemical Physics, 2005, 122, 044110.	1.2	157
1973	Variational grand-canonical electronic structure method for open systems. Journal of Chemical Physics, 2005, 123, 044112.	1.2	12
1974	Atomic layer deposition of high- $\hat{\epsilon}$ dielectrics on nitrided silicon surfaces. Applied Physics Letters, 2005, 86, 192110.	1.5	15
1975	Density Functional Theory with Correct Long-Range Asymptotic Behavior. Physical Review Letters, 2005, 94, 043002.	2.9	372
1976	Quantum Mechanical Free Energy Barrier for an Enzymatic Reaction. Physical Review Letters, 2005, 94, 138302.	2.9	136
1977	Efficient exact exchange approximations in density-functional theory. Journal of Chemical Physics, 2005, 123, 164116.	1.2	27

#	ARTICLE	IF	CITATIONS
1978	Linear scaling computation of the Fock matrix. VII. Periodic density functional theory at the Γ point. <i>Journal of Chemical Physics</i> , 2005, 122, 134102.	1.2	11
1979	Positively charged carbon vacancy in three inequivalent lattice sites of $6H\alpha$ -SiC: Combined EPR and density functional theory study. <i>Physical Review B</i> , 2005, 71, .	1.1	26
1980	Analytic energy gradients of the optimized effective potential method. <i>Journal of Chemical Physics</i> , 2005, 123, 134111.	1.2	12
1981	Quantifying the effects of the self-interaction error in DFT: When do the delocalized states appear?. <i>Journal of Chemical Physics</i> , 2005, 122, 224103.	1.2	230
1982	Time-dependent density-functional theory calculations of triplet-triplet absorption. <i>Journal of Chemical Physics</i> , 2005, 122, 224104.	1.2	12
1983	^{29}Si NMR Chemical Shift Calculation for Silicate Species by Gaussian Software. <i>Journal of the Physical Society of Japan</i> , 2005, 74, 1609-1620.	0.7	40
1984	Selective Adsorption of Organosulfur Compounds from Transportation Fuels by Cu^{II} -Complexation. <i>Separation Science and Technology</i> , 2005, 39, 1717-1732.	1.3	49
1985	Molecular dynamics study of lignin constituents in water. <i>Holzforschung</i> , 2005, 59, 253-262.	0.9	9
1986	A Theoretical Study on the Reaction Mechanism for the Bergman Cyclization from the Perspective of the Electron Localization Function and Catastrophe Theory. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3687-3693.	1.1	57
1987	Progress in the development of exchange-correlation functionals. , 2005, , 669-724.		108
1988	Interrelation between H-Bond and π -Electron Delocalization. <i>Chemical Reviews</i> , 2005, 105, 3513-3560.	23.0	622
1989	The performance of hybrid density functionals in solid state chemistry: the case of BaTiO_3 . <i>Molecular Physics</i> , 2005, 103, 2483-2496.	0.8	141
1990	Structures and electron affinities of the di-arsenic fluorides $\text{As}_2\text{F}_n/\text{As}_2\text{F}_n^-$ ($n= 1-8$). <i>Journal of Computational Chemistry</i> , 2005, 26, 411-435.	1.5	5
1991	Periodic Trends in Bond Dissociation Energies. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4359-4365.	1.1	67
1992	Steric Effects in Metathesis and Reduction Reactions of Phosphinimines with Catechol- and Pinacolboranes. <i>Inorganic Chemistry</i> , 2005, 44, 4301-4308.	1.9	31
1993	Solid-State ^{13}C NMR and DFT Quantum-Chemical Study of Polymer Electrolyte Poly(2-ethyl-2-oxazoline)/ AgCF_3SO_3 . <i>Macromolecules</i> , 2005, 38, 5083-5087.	2.2	6
1994	Density functional calculations of molecular parity-violating effects within the zeroth-order regular approximation. <i>Journal of Chemical Physics</i> , 2005, 122, 134316.	1.2	43
1995	A density-functional-theory study of atomic nitrogen abstraction from $\text{Si}(100)-(2\times 1)$ by a gaseous $\text{O}(\text{P}3)$ atom. <i>Journal of Chemical Physics</i> , 2005, 122, 234705.	1.2	1

#	ARTICLE	IF	CITATIONS
1996	Ground- and excited-state electronic structure of an iron-containing molecular spin photoswitch. <i>Journal of Chemical Physics</i> , 2005, 123, 094709.	1.2	9
1997	Dissolution nature of the lithium hydroxide by water molecules. <i>Journal of Chemical Physics</i> , 2005, 123, 084321.	1.2	25
1998	Vibrational and electronic structure of the dinuclear bis(μ -nitrido) vanadium(v) complex $[V(N\{\hat{N}\}^3)_2(\hat{\mu}\text{-N})_2]$: spectroscopic properties of the $M_2(\hat{\mu}\text{-N})_2$ diamond core. <i>Dalton Transactions</i> , 2005, , 1052-1057.	1.6	16
1999	Tetramethylcyclopentadienylselenium derivatives. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 3990.	1.5	6
2000	Hydrogen formation in the reaction of $Zn^+(H_2O)_n$ with HCl. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 981.	1.3	17
2001	Theoretical Study of the Antioxidant Activity of Vitamin E: Reactions of \hat{I}^\pm -Tocopherol with the Hydroperoxy Radical. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 337-344.	2.3	32
2002	Thermal Decomposition of the Perfluorinated Peroxides $CF_3OC(O)OOC(O)F$ and $CF_3OC(O)OOCF_3$. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7481-7488.	1.1	5
2003	Coordination properties of glycylglycine to Cu^+ , Ni^+ and Co^+ . Influence of metal cation electronic configuration. <i>New Journal of Chemistry</i> , 2005, 29, 1585.	1.4	32
2004	A computational study of the reactions of a \hat{I}^2 -diketiminatoaluminium(i) complex with the hydrogen atom and the electron. <i>Chemical Communications</i> , 2005, , 1134-1136.	2.2	8
2005	$IrII(\text{ethene})$: Metal or carbon radical? Part II: Oxygenation via iridium or direct oxygenation at ethene?. <i>Dalton Transactions</i> , 2005, , 979.	1.6	40
2006	Synthesis of an IGD peptidomimetic with motogenic activity. <i>Molecular BioSystems</i> , 2005, 1, 318.	2.9	3
2007	A CCSD estimation of the $O\hat{C}H$ bond dissociation enthalpies of pyrogallol. <i>New Journal of Chemistry</i> , 2005, 29, 535-537.	1.4	10
2008	Electron affinities of the radicals derived from cytosine. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 861.	1.3	23
2009	Electronic effect of different positions of the $\hat{C}NO_2$ group on the DNA-intercalator of chiral complexes $[Ru(\text{bpy})_2L]^{2+}$ ($L = o\text{-npip}$, $m\text{-npip}$ and $p\text{-npip}$). <i>Dalton Transactions</i> , 2005, , 2038.	1.6	84
2010	A widely applicable concept for predictable induction of preferred configuration in C_3 -symmetric systems. <i>Chemical Communications</i> , 2005, , 2799.	2.2	46
2011	Novel bromine oxyfluorides: structures, thermochemistry and electron affinities of $BrOF_n/BrO$ ($n = 1-5$). <i>Molecular Physics</i> , 2005, 103, 1995-2008.	0.8	6
2012	Gas-Phase Structure of Protonated Histidine and Histidine Methyl Ester: Combined Experimental Mass Spectrometry and Theoretical ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8329-8335.	1.1	33
2013	Multi-coefficient extrapolated density functional theory for thermochemistry and thermochemical kinetics. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 43.	1.3	393

#	ARTICLE	IF	CITATIONS
2014	Modeling Acid and Cationic Catalysis on the Reactivity of Duocarmycins. <i>Journal of Organic Chemistry</i> , 2005, 70, 7098-7106.	1.7	10
2015	Explaining the Effects of Tâˆ”Oâˆ”T Bond Angles on NMR Chemical Shifts in Aluminosilicates: A Natural Bonding Orbital (NBO) and Natural Chemical Shielding (NCS) Analysis. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3060-3066.	1.1	24
2016	Interpretation of Conformational Effects on 2-endo-Norborneol by Natural Chemical Shielding Analysis. <i>Journal of Physical Chemistry A</i> , 2005, 109, 802-806.	1.1	4
2017	Synthesis and Characterization of a Novel Terthiophene-Based Quinodimethane Bearing a 3,4-Ethylenedioxythiophene Central Unit. <i>Journal of Physical Chemistry B</i> , 2005, 109, 22308-22318.	1.2	18
2018	Combined Quantum Mechanical/Molecular Mechanical Study on the Pentacoordinated Ferric and Ferrous Cytochrome P450cam Complexes. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1268-1280.	1.2	60
2019	A Theoretical Study on the Electronic Structures of TiO ₂ : A Effect of Hartree-Fock Exchange. <i>Journal of Physical Chemistry B</i> , 2005, 109, 19270-19277.	1.2	135
2020	Synthesis of the Five-Coordinate Ruthenium(II) Complexes [(PCP)Ru(CO)(L)] [BAr ⁴] {PCP = 2,6-(CH ₂ PrBu ₂) ₂ C ₆ H ₃ , BAr ⁴ = 3,5-(CF ₃) ₂ C ₆ H ₃ , L = 1-ClCH ₂ Cl, 1-1-N ₂ , or 1/4-Clâˆ”Ru(PCP)(CO)}: Reactions with Phenyl diazomethane and Phenylacetylene. <i>Inorganic Chemistry</i> , 2005, 44, 8379-8390.		25
2021	Inductive Effect-Assisted Chain-Growth Polycondensation. Synthetic Development from para-to meta-Substituted Aromatic Polyamides with Low Polydispersities. <i>Journal of the American Chemical Society</i> , 2005, 127, 10172-10173.	6.6	68
2022	Assessing Alkyl-, Silyl-, and Halo-Substituent Effects on the Electron Affinities of Silyl Radicals. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10100-10105.	1.1	4
2023	Adiabatic Electron Affinities of the Polyhydrated Adenine-Thymine Base Pair: A Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3971-3979.	1.1	43
2024	Chiral Zirconium Catalysts Using Multidentate BINOL Derivatives for Catalytic Enantioselective Mannich-Type Reactions; Ligand Optimization and Approaches to Elucidation of the Catalyst Structure. <i>Journal of the American Chemical Society</i> , 2005, 127, 15528-15535.	6.6	54
2025	Quantum Chemical Evaluation of Protein Control over Heme Ligation: CO/O ₂ Discrimination in Myoglobin. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3065-3070.	1.2	51
2026	Electrostatic DFT Map for the Complete Vibrational Amide Band of NMA. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9747-9759.	1.1	180
2027	The Electronic Structure of Inorganic Benzenes: Valence Bond and Ring-Current Descriptions. <i>Inorganic Chemistry</i> , 2005, 44, 5266-5272.	1.9	71
2028	Koopmans-like Approximation in the Kohn-Sham Method and the Impact of the Frozen Core Approximation on the Computation of the Reactivity Parameters of the Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8880-8892.	1.1	44
2029	Proximity Effects in the Palladium-Catalyzed Substitution of Aryl Fluorides. <i>Organic Letters</i> , 2005, 7, 1011-1014.	2.4	43
2030	Dissociation of Benzene Dication [C ₆ H ₆] ²⁺ : Exploring the Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11551-11559.	1.1	27
2031	Conformationally Gated Switching between Superexchange and Hopping within Oligo-p-phenylene-Based Molecular Wires. <i>Journal of the American Chemical Society</i> , 2005, 127, 11842-11850.	6.6	171

#	ARTICLE	IF	CITATIONS
2032	Kinetics of the Unimolecular Decomposition of the 2-Chloroallyl Radical. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8149-8157.	1.1	4
2033	A theoretical study of the structures and stabilities of N ₄ O ₂ isomers. <i>Molecular Physics</i> , 2005, 103, 249-256.	0.8	0
2034	Glycolaldehyde + OH Gas Phase Reaction: A Quantum Chemistry + CVT/SCT Approach. <i>Journal of Physical Chemistry A</i> , 2005, 109, 169-180.	1.1	65
2035	Synthesis and Reactivity of Molybdenum(IV) Complexes with Alkyl and Aryl Isocyanides. <i>Organometallics</i> , 2005, 24, 6310-6318.	1.1	8
2036	Slater's Exchange Parameters \hat{I}_{\pm} for Analytic and Variational $X\hat{I}_{\pm}$ Calculations. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1193-1200.	2.3	19
2037	Silicon Monohydride Clusters SinH (n = 4-10) and Their Anions: Structures, Thermochemistry, and Electron Affinities. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5717-5723.	1.1	19
2038	Effects of Fluorine on the Structures and Energetics of the Propynyl and Propargyl Radicals and Their Anions. <i>Journal of Organic Chemistry</i> , 2005, 70, 8676-8686.	1.7	10
2039	Probing Structure in the Polymorphic Domain of the l-Enantiomer of N-Benzoyl-Phenylalanine by Means of 2D Solid-State NMR Spectroscopy and DFT Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23175-23182.	1.2	11
2040	Between Ni(mnt) ₂ and Ni(tfd) ₂ Dithiolene Complexes: The Unsymmetrical 2-(Trifluoromethyl)acrylonitrile-1,2-dithiolate and Its Nickel Complexes. <i>Inorganic Chemistry</i> , 2005, 44, 9763-9770.	1.9	42
2041	Comparative DFT Study of the Spin Trapping of Methyl, Mercapto, Hydroperoxy, Superoxide, and Nitric Oxide Radicals by Various Substituted Cyclic Nitrones. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1662-1674.	1.1	36
2042	Synthesis and Characterization of Three Novel Perfluoro-oligothiophenes Ranging in Length from the Trimer to the Pentamer. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20737-20745.	1.2	16
2043	Influence of Cu ⁺ on the RS-NO Bond Dissociation Energy of S-Nitrosothiols. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1334-1336.	1.2	34
2044	Computational Evaluation of the Evidence for Tri-trans-[12]Annulene. <i>Journal of Organic Chemistry</i> , 2005, 70, 3602-3609.	1.7	38
2045	PCM Study of the Solvent and Substituent Effects on the Conformers, Intramolecular Hydrogen Bonds and Bond Dissociation Enthalpies of 2-Substituted Phenols. <i>Journal of Physical Chemistry A</i> , 2005, 109, 366-377.	1.1	42
2046	The Mechanism of Proton Transfer between Adjacent Sites Exposed to Water. <i>Journal of Physical Chemistry B</i> , 2005, 109, 11379-11388.	1.2	22
2047	Calculation of Electron Detachment Energies for Water Cluster Anions: An Appraisal of Electronic Structure Methods, with Application to (H ₂ O) ₂₀ - and (H ₂ O) ₂₄ -. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5217-5229.	1.1	139
2048	An ab initio study of the hyperfine structure in the X ² Σ ⁻ electronic state of HCCS: calculation of vibrationally averaged components of the anisotropic hyperfine tensor. <i>Molecular Physics</i> , 2005, 103, 587-598.	0.8	5
2049	Structures and Thermochemistry of Calcium-Containing Molecules. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9156-9168.	1.1	17

#	ARTICLE	IF	CITATIONS
2050	Theoretical Study of the Human DNA Repair Protein HOGG1 Activity. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1713-1719.	1.1	38
2051	Electronic and Structural Evolution and Chemical Bonding in Tungsten Oxide Clusters: W_2O_n and $W_2O_n(n=1\sim 6)$. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6019-6030.	1.1	67
2052	Density Functional Study of AuX_q ($X = O, S, Se, Te, q = +1, 0, \sim 1$) Molecules. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5951-5955.	1.1	13
2053	Radical Hydrometalation of Functional Ethylenic Compounds: Radical Autoinhibition Changes the Regioselectivity. <i>Organometallics</i> , 2005, 24, 446-454.	1.1	8
2054	$IrI(ethene)$: Metal or Carbon Radical?. <i>Journal of the American Chemical Society</i> , 2005, 127, 1895-1905.	6.6	76
2055	Thermochemical Properties, Rotation Barriers, and Group Additivity for Unsaturated Oxygenated Hydrocarbons and Radicals Resulting from Reaction of Vinyl and Phenyl Radical Systems with O_2 . <i>Journal of Physical Chemistry A</i> , 2005, 109, 2233-2253.	1.1	37
2056	Design of Density Functionals That Are Broadly Accurate for Thermochemistry, Thermochemical Kinetics, and Nonbonded Interactions. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5656-5667.	1.1	1,451
2057	Comparative Study of the Bonding in the First Series of Transition Metal 1:1 Complexes $M\sim L$ ($M = Sc, \dots$). <i>J. Phys. Chem. A</i> , 2005, 109, 7843-7855.	1.1	14
2058	Toward an Understanding of the Catalytic Role of Hydrogen-Bond Donor Solvents in the Hetero-Diels-Alder Reaction between Acetone and Butadiene Derivative. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10438-10444.	1.1	43
2059	Enantioselective Nonsteroidal Aromatase Inhibitors Identified through a Multidisciplinary Medicinal Chemistry Approach. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 7282-7289.	2.9	64
2060	Theoretical Methods of Potential Use for Studies of Inorganic Reaction Mechanisms. <i>Chemical Reviews</i> , 2005, 105, 2695-2722.	23.0	387
2061	Electronic Structure Studies of the Adenosylcobalamin Cofactor in Glutamate Mutase. <i>Biochemistry</i> , 2005, 44, 15167-15181.	1.2	28
2062	Infrared Spectra of a Species of Astrochemical Interest: Aminoacrylonitrile (3-Amino-2-propenenitrile). <i>Journal of Physical Chemistry A</i> , 2005, 109, 4705-4712.	1.1	22
2063	Probing the Geometric and Electronic Structures of the Low-Temperature Azide Adduct and the Product-Inhibited Form of Oxidized Manganese Superoxide Dismutase. <i>Biochemistry</i> , 2005, 44, 1504-1520.	1.2	57
2064	A Comparison of the Cope Rearrangements of cis-1,2-Divinylicyclopropane, cis-2,3-Divinylaziridine, cis-2,3-Divinyloxirane, cis-2,3-Divinyolphosphirane, and cis-2,3-Divinyllthiirane: A DFT Study. <i>Journal of Organic Chemistry</i> , 2005, 70, 6018-6026.	1.7	34
2065	Coordination Properties of the Oxime Analogue of Glycine to Cu(II). <i>Journal of Physical Chemistry A</i> , 2005, 109, 5668-5676.	1.1	46
2066	Removing Critical Errors for DFT Applications to Transition-Metal Nanoclusters: Correct Ground-State Structures of Ru Clusters. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23113-23117.	1.2	43
2067	Density Functional Theoretical Study of a Series of Binary Azides $M(N_3)_n$ ($n = 3, 4$). <i>Journal of Physical Chemistry A</i> , 2005, 109, 9089-9094.	1.1	20

#	ARTICLE	IF	CITATIONS
2068	157 nm Pellicles (Thin Films) for Photolithography: A Mechanistic Investigation of the VUV and UV-C Photolysis of Fluorocarbons. <i>Journal of the American Chemical Society</i> , 2005, 127, 8320-8327.	6.6	12
2069	Theoretical Study of the Suicide Inhibition Mechanism of the Enzyme Pyruvate Formate Lyase by Methacrylate. <i>Journal of the American Chemical Society</i> , 2005, 127, 6902-6909.	6.6	8
2070	Density functional theory study of MnO by a hybrid functional approach. <i>Physical Review B</i> , 2005, 72, .	1.1	160
2071	Alternated Quinoid/Aromatic Units in Terthiophenes Building Blocks for Electroactive Narrow Band Gap Polymers. Extended Spectroscopic, Solid State, Electrochemical, and Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 16616-16627.	1.2	48
2072	Conversions of Ruthenium(III) Alkyl Complexes to Ruthenium(II) through Ru-Calkyl Bond Homolysis. <i>Organometallics</i> , 2005, 24, 1301-1305.	1.1	23
2073	σ-Type ethane adsorption complexes with Cu ⁺ ions in Cu(I)-ZSM-5 zeolite. Combined DRIFTS and DFT study. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 1939-1944.	1.3	29
2074	Cross-Linking between Thymine and Indolyl Radical: A Possible Mechanisms for Cross-Linking of DNA and Tryptophan-Containing Peptides. <i>Bioconjugate Chemistry</i> , 2005, 16, 588-597.	1.8	10
2075	Trapping of the OH Radical by α-Tocopherol: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4777-4784.	1.1	39
2076	Metal versus Ligand Alkylation in the Reactivity of the (Bis-iminopyridinato)Fe Catalyst. <i>Journal of the American Chemical Society</i> , 2005, 127, 13019-13029.	6.6	107
2077	The electronic spectrum of protonated adenine: Theory and experiment. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3306.	1.3	96
2078	Benchmark Database of Barrier Heights for Heavy Atom Transfer, Nucleophilic Substitution, Association, and Unimolecular Reactions and Its Use to Test Theoretical Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2012-2018.	1.1	736
2079	Conjugated Polymers and Aromaticity. <i>Chemical Reviews</i> , 2005, 105, 3448-3481.	23.0	447
2080	β-Lactam antibiotics are multipotent agents to combat neurological diseases. <i>Biochemical and Biophysical Research Communications</i> , 2005, 333, 661-663.	1.0	40
2081	Theoretical investigation of iron isotope fractionation between Fe(H ₂ O) ₆ ³⁺ and Fe(H ₂ O) ₆ ²⁺ : Implications for iron stable isotope geochemistry. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 825-837.	1.6	219
2082	ATR-FTIR spectroscopic characterization of coexisting carbonate surface complexes on hematite. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 1527-1542.	1.6	166
2083	Structural and electronic properties of 3,4-ethylenedioxythiophene, 3,4-ethylenedisulfanylfurane and thiophene oligomers: A theoretical investigation. <i>Synthetic Metals</i> , 2005, 149, 151-156.	2.1	50
2084	A theoretical study of the effects produced by N-hydroxyalkyl substitution in pyrrole oligomers. <i>Synthetic Metals</i> , 2005, 151, 239-245.	2.1	12
2085	A mechanism for carbon isotope exchange between aqueous acetic acid and : An ab initio study. <i>Organic Geochemistry</i> , 2005, 36, 835-850.	0.9	11

#	ARTICLE	IF	CITATIONS
2086	Insights into the structure of cutin and cutan from <i>Agave americana</i> leaf cuticle using HRMAS NMR spectroscopy. <i>Organic Geochemistry</i> , 2005, 36, 1072-1085.	0.9	102
2087	A direct method for locating minimum-energy crossing points (MECPs) in spin-forbidden transitions and nonadiabatic reactions. <i>Journal of Chemical Physics</i> , 2005, 123, 094711.	1.2	46
2088	Prediction of the Formation and Stabilities of Energetic Salts and Ionic Liquids Based on ab Initio Electronic Structure Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23196-23208.	1.2	141
2089	Effect of Heteroatom Insertion at the Side Chain of 5-Alkyl-1H-tetrazoles on Their Properties as Catalysts for Ester Hydrolysis at Neutral pH. <i>Journal of Organic Chemistry</i> , 2005, 70, 9677-9685.	1.7	29
2090	Time-dependent density functional theory: Past, present, and future. <i>Journal of Chemical Physics</i> , 2005, 123, 062206.	1.2	791
2091	Molecular Modeling of the Short-Side-Chain Perfluorosulfonic Acid Membrane. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7583-7593.	1.1	194
2092	Characterization of a 1:1 Cu ²⁺ O ₂ Adduct Supported by an Anilido Imine Ligand. <i>Inorganic Chemistry</i> , 2005, 44, 6989-6997.	1.9	90
2093	Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions. <i>Journal of Chemical Physics</i> , 2005, 123, 161103.	1.2	979
2094	Theoretical Study on the Electronic Structure and Optical Properties of Mercury-Containing Diethynylfluorene Monomer, Oligomer, and Polymer. <i>Organometallics</i> , 2005, 24, 385-394.	1.1	30
2095	Where Is the Spin? Understanding Electronic Structure and g-Tensors for Ruthenium Complexes with Redox-Active Quinonoid Ligands. <i>Journal of the American Chemical Society</i> , 2005, 127, 11399-11413.	6.6	164
2096	The Peculiar Trend of Cyclic Perfluoroalkane Electron Affinities with Increasing Ring Size. <i>Journal of the American Chemical Society</i> , 2005, 127, 15457-15469.	6.6	29
2097	Tautomers and electronic states of jet-cooled 2-aminopurine investigated by double resonance spectroscopy and theory. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3021.	1.3	59
2098	The ¹⁷ O Hyperfine Interaction in V ¹⁷ O(H ²¹⁷ O) ₅ ²⁺ and Mn(H ²¹⁷ O) ₆ ²⁺ Determined by High Field ENDOR Aided by DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7865-7871.	1.1	51
2099	Energy band gaps and lattice parameters evaluated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. <i>Journal of Chemical Physics</i> , 2005, 123, 174101.	1.2	1,604
2100	N ₄ Ring as a Square Planar Ligand in Novel MN ₄ Species. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3182-3186.	1.1	20
2101	Copper ²⁺ /Zinc Superoxide Dismutase: A Theoretical Insights into the Catalytic Mechanism. <i>Inorganic Chemistry</i> , 2005, 44, 3311-3320.	1.9	86
2102	Insertion of noble-gas atom (Kr and Xe) into noble-metal molecules (AuF and AuOH): Are they stable?. <i>Journal of Chemical Physics</i> , 2005, 123, 074323.	1.2	74
2103	Optimized Spin Crossings and Transition States for Short-range Electron Transfer in Transition Metal Dimers. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10513-10520.	1.2	15

#	ARTICLE	IF	CITATIONS
2104	Raman and Theoretical Study of the Solvent Effects on the Sizable Intramolecular Charge Transfer in the Push~Pull 5-(Dimethylamino)-5-~nitro-2,2~bithiophene. Journal of Physical Chemistry A, 2005, 109, 8724-8731.	1.1	28
2105	Incisive Structure~Spectroscopic Correlation in Oligothiophenes Functionalized with ($\hat{\Delta}$) Inductive/Mesomeric Fluorine Groups:~Joint Raman and DFT Study. Journal of the American Chemical Society, 2005, 127, 13364-13372.	6.6	29
2106	The Structure of Active Centers and the Ethylene Polymerization Mechanism on the Cr/SiO ₂ Catalyst:~A Frontier for the Characterization Methods. Chemical Reviews, 2005, 105, 115-184.	23.0	396
2107	Hypervalent ammonium radicals. Competitive N~C and N~H bond dissociations in methyl ammonium and ethyl ammonium. Physical Chemistry Chemical Physics, 2005, 7, 912-920.	1.3	35
2108	Gold behaves as hydrogen: Prediction on the existence of a new class of boron-containing radicals, AuBX (X=F,Cl,Br). Journal of Chemical Physics, 2005, 123, 241101.	1.2	22
2109	Potential Energy Surface Profile of the Oxygen Reduction Reaction on a Pt Cluster:~Adsorption and Decomposition of OOH and H ₂ O ₂ . Journal of Chemical Theory and Computation, 2005, 1, 935-943.	2.3	60
2110	Role of Hartree~Fock and Kohn~Sham Orbitals in the Basis Set Superposition Error for Systems Linked by Hydrogen Bonds. Journal of Physical Chemistry A, 2005, 109, 643-651.	1.1	22
2111	Density Functional Methods for Excited States: Equilibrium Structure and Electronic Spectra. Theoretical and Computational Chemistry, 2005, 16, 93-128.	0.2	192
2112	The quadrupole moment of the 3~ ²⁺ nuclear ground state of Au ¹⁹⁷ from electric field gradient relativistic coupled cluster and density-functional theory of small molecules and the solid state. Journal of Chemical Physics, 2005, 122, 124317.	1.2	37
2113	Role of Donor~Acceptor Strengths and Separation on the Two-Photon Absorption Response of Cytotoxic Dyes:~A TD-DFT Study. Journal of Physical Chemistry A, 2005, 109, 7276-7284.	1.1	55
2114	Sterically Controlled Esterification on Bis($\hat{1}/4$ -hydroxo) Dioxovanadium Site in $\hat{1}^3$ -H ₂ SiV ₂ W ₁₀ O ₄₀ -. Inorganic Chemistry, 2005, 44, 14-16.	1.9	37
2115	Reactivity of Bis($\hat{1}/4$ -hydroxo) Divanadium Site in $\hat{1}^3$ -H ₂ SiV ₂ W ₁₀ O ₄₀ - with Hydroxo Compounds. Inorganic Chemistry, 2005, 44, 9068-9075.	1.9	34
2116	A new pathway for the rapid decay of electronically excited adenine. Journal of Chemical Physics, 2005, 122, 104314.	1.2	217
2117	Molecular Modeling and Chemical Reactivity of Sanfetrinem and Derivatives. Journal of Physical Chemistry B, 2005, 109, 9780-9786.	1.2	2
2118	Reliability of the density functional approximation to describe the charge transfer and electrostatic complexes involved in the modeling of organic conducting polymers. Physical Review E, 2005, 72, 026704.	0.8	15
2119	Relativistic two-component calculations of electronic g-tensors that include spin polarization. Journal of Chemical Physics, 2005, 123, 244103.	1.2	72
2120	Design of Oxygen Reduction Bimetallic Catalysts:~Ab-Initio-Derived Thermodynamic Guidelines. Journal of Physical Chemistry B, 2005, 109, 18902-18906.	1.2	175
2121	The electronic structure of free water clusters probed by Auger electron spectroscopy. Journal of Chemical Physics, 2005, 123, 054310.	1.2	80

#	ARTICLE	IF	CITATIONS
2122	Theoretical Investigation on the Rotational Isomerism of Calix[4]arenes: Influence of the Hydroxyl and Methoxy Replacement. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8049-8054.	1.1	19
2123	(E)/(Z) Selectivity in the Polymerization of 2-Butene Promoted by Ni(II) Brookhart-Type Catalysts. <i>Macromolecules</i> , 2005, 38, 2072-2075.	2.2	16
2124	Möbius Aromaticity in [12]Annulene: Cis-Trans Isomerization via Twist-Coupled Bond Shifting. <i>Journal of the American Chemical Society</i> , 2005, 127, 9704-9705.	6.6	65
2125	Mesitylthio-Oligothiophenes in Various Redox States. Molecular and Electronic Views as Offered by Spectroscopy and Theory. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11275-11284.	1.1	21
2126	Liquid Crystalline Metal-Free Phthalocyanines Designed for Charge and Exciton Transport. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20315-20323.	1.2	101
2127	The Perfluoroadamantyl Radicals C10F15 and Their Anions. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 279-285.	2.3	1
2128	Perfluoroadamantane and Its Negative Ion. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1454-1457.	1.1	11
2129	The mechanism for dioxygen formation in PSII studied by quantum chemical methods. <i>Photochemical and Photobiological Sciences</i> , 2005, 4, 1035.	1.6	68
2130	Interaction of Co ⁺ and Co ²⁺ with Glycine. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 224-230.	1.1	42
2131	Theoretical Study of Singlet and Triplet Excitation Energies in Oligothiophenes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3078-3085.	1.1	73
2132	Efficient evaluation of short-range Hartree-Fock exchange in large molecules and periodic systems. <i>Journal of Chemical Physics</i> , 2006, 125, 104103.	1.2	200
2133	Importance of short-range versus long-range Hartree-Fock exchange for the performance of hybrid density functionals. <i>Journal of Chemical Physics</i> , 2006, 125, 074106.	1.2	823
2134	Energy and Electron Transfer in β^2 -Alkynyl-Linked Porphyrin-[60]Fullerene Dyads. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14155-14166.	1.2	100
2135	Gas-Phase DNA Oligonucleotide Structures. A QM/MM and Atoms in Molecules Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3992-4000.	1.1	52
2136	ansa-Chromocene Complexes. 2. Isocyanide Derivatives of Cr(II) and Cr(III), Their Syntheses, X-ray Crystal Structures, and Physical Properties. <i>Organometallics</i> , 2006, 25, 719-732.	1.1	25
2137	Substituent Effects on Enthalpies of Formation of Nitrogen Heterocycles: 2-Substituted Benzimidazoles and Related Compounds. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2535-2544.	1.1	17
2138	Nitro Group as a Means of Attaching Organic Molecules to Silicon: Nitrobenzene on Si(100)-2 \times 1. <i>Journal of Physical Chemistry B</i> , 2006, 110, 6899-6905.	1.2	26
2139	A study of the radical-radical reaction dynamics of O(P3)+t-C4H9OH+iso-C4H8. <i>Journal of Chemical Physics</i> , 2006, 124, 104307.	1.2	17

#	ARTICLE	IF	CITATIONS
2140	Adsorption and Dissociation of H ₂ O ₂ on Pt and Pt ⁺ Alloy Clusters and Surfaces. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17452-17459.	1.2	76
2141	Theoretical Study of Free-Radical-Mediated 5-exo-Trig Cyclizations of Chiral 3-Substituted Hepta-1,6-dienes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3714-3722.	1.1	8
2142	Dynamic Processes in [16]Annulene: M ⁺ Bond-Shifting Routes to Configuration Change. <i>Journal of the American Chemical Society</i> , 2006, 128, 16692-16700.	6.6	35
2143	[10]Annulene: Bond Shifting and Conformational Mechanisms for Automerization. <i>Journal of Organic Chemistry</i> , 2006, 71, 3001-3006.	1.7	25
2144	Structural and Electronic Differences of Copper(I) Complexes with Tris(pyrazolyl)methane and Hydrotris(pyrazolyl)borate Ligands. <i>Inorganic Chemistry</i> , 2006, 45, 1698-1713.	1.9	127
2145	Experimental and Theoretical Investigations of IR Spectra and Electronic Structures of the U(OH) ₂ , UO ₂ (OH), and UO ₂ (OH) ₂ Molecules. <i>Inorganic Chemistry</i> , 2006, 45, 4157-4166.	1.9	23
2146	CP/MAS13C NMR Characterization of the Isomeric States and Intermolecular Packing in Tris(8-hydroxyquinoline) Aluminum(III) (Alq ₃). <i>Journal of the American Chemical Society</i> , 2006, 128, 4292-4297.	6.6	73
2147	Aminophosphonates as organocatalysts in the direct asymmetric aldol reaction: towards syn selectivity in the presence of Lewis bases. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 2091-2096.	1.5	74
2148	Microwave Spectrum, Structure, and Quantum Chemical Studies of a Compound of Potential Astrochemical and Astrobiological Interest: β -3-Amino-2-propenenitrile. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12572-12584.	1.1	25
2149	Spectroscopic and Computational Studies on the Coordination-Driven Self-Assembly Complexes (ZnL) ₂ and (NiL) ₂ [L = Bis(2,4-dimethyldipyrrin-3-yl)methane]. <i>Journal of Physical Chemistry B</i> , 2006, 110, 21958-21965.	1.2	28
2150	Stabilization of the tautomers HP(OH) ₂ and P(OH) ₃ of hypophosphorous and phosphorous acids as ligands. <i>Dalton Transactions</i> , 2006, , 389-395.	1.6	50
2151	Comparative assessment of density functional methods for 3d transition-metal chemistry. <i>Journal of Chemical Physics</i> , 2006, 124, 224105.	1.2	180
2152	Towards understanding performance differences between approximate density functionals for spin states of iron complexes. <i>Journal of Chemical Physics</i> , 2006, 125, 174102.	1.2	44
2153	Cycloaddition Functionalizations to Preserve or Control the Conductance of Carbon Nanotubes. <i>Physical Review Letters</i> , 2006, 97, 116801.	2.9	133
2154	Canonical Watson-Crick base pair interactions in π - π^* type triplet states. <i>Molecular Physics</i> , 2006, 104, 925-931.	0.8	5
2155	SPOCK.Cl: A multireference spin-orbit configuration interaction method for large molecules. <i>Journal of Chemical Physics</i> , 2006, 124, 124101.	1.2	105
2156	Investigation of a localised second-order Brueckner correlation method. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 563-572.	1.3	11
2157	Encapsulation of metal cations and anions within the cavity of bis(1,4,7-triazacyclononane) receptors. <i>Dalton Transactions</i> , 2006, , 1409-1418.	1.6	23

#	ARTICLE	IF	CITATIONS
2158	N π -N splitting of a functionalized μ -1:1-coordinated N ₂ ligand leading to a μ -nitrido μ -imido core: mechanistic insight from DFT. Dalton Transactions, 2006, , 1137-1140.	1.6	18
2159	Mononuclear metavanadate catalyses gas phase oxidation of methanol to formaldehyde employing dioxygen as the terminal oxidant. Chemical Communications, 2006, , 4503.	2.2	43
2160	P-Heterocyclic carbenes as potential ligands in the design of new metathesis catalysts. A computational study. Dalton Transactions, 2006, , 2214.	1.6	15
2161	Exact energy expression in the strong-interaction limit of the density functional theory. Philosophical Magazine, 2006, 86, 2101-2114.	0.7	2
2162	Ab initio study of hydrated sodium halides NaX(H ₂ O) ₆ (X=F, Cl, Br, and I). Journal of Chemical Physics, 2006, 124, 024321.	1.2	82
2163	Direct influence of hydrogen-bonding on the reduction potential of a CuII center. Chemical Communications, 2006, , 1024.	2.2	17
2164	Ab initio rigid water: Effect on water structure, ion hydration, and thermodynamics. Physical Chemistry Chemical Physics, 2006, 8, 2153.	1.3	33
2165	Computational study on reactivity of cyclic organometallic dienes containing silicon, germanium and tin. New Journal of Chemistry, 2006, 30, 1149.	1.4	9
2166	Structural and conformational study of two solvates of a fulgenic acid derivative. New Journal of Chemistry, 2006, 30, 647.	1.4	1
2167	Kinetics and mechanism of the β -alanine + OH gas phase reaction: A quantum mechanical approach. Physical Chemistry Chemical Physics, 2006, 8, 285-292.	1.3	15
2168	Density-Functional Theory Investigation of the Geometric, Energetic, and Optical Properties of the Cobalt(II)tris(2,2'-bipyridine) Complex in the High-Spin and the Jahn-Teller Active Low-Spin States. Journal of Chemical Theory and Computation, 2006, 2, 1342-1359.	2.3	52
2169	Silicon Hydride Clusters Si ₅ H _n (n = 3-12) and Their Anions: Structures, Thermochemistry, and Electron Affinities. Journal of Physical Chemistry A, 2006, 110, 12026-12034.	1.1	27
2170	Octahedral [TpRu(PMe ₃) ₂ OR] _n Complexes (Tp = hydridotris(pyrazolyl)borate; R = H or Ph; n = 0 or 1): Reactions at Ru(II) and Ru(III) Oxidation States with Substrates that Possess Carbon-Hydrogen Bonds. Organometallics, 2006, 25, 5456-5465.	1.1	29
2171	Facilitating Access to the Most Easily Ionized Molecule: an Improved Synthesis of the Key Intermediate, W ₂ (hpp) ₄ Cl ₂ , and Related Compounds. Inorganic Chemistry, 2006, 45, 201-213.	1.9	40
2172	Radical Ions of β -Bis(diphenylamino)-capped Oligothiophenes: A Combined Spectroelectrochemical and Theoretical Study. Journal of Physical Chemistry B, 2006, 110, 8223-8231.	1.2	46
2173	Molecular dynamics DFT:B3LYP study of guanosinetriphosphate conversion into guanosinemonophosphate upon Mg ²⁺ chelation of α and β phosphate oxygens of the triphosphate tail. Physical Chemistry Chemical Physics, 2006, 8, 2187.	1.3	12
2174	Can an ancillary ligand lead to a thermodynamically stable end-on 1 : 1 Cu ^{II} -O ₂ adduct supported by a β -diketiminato ligand?. Dalton Transactions, 2006, , 4773-4782.	1.6	12
2175	Assessing a new nonempirical density functional: Difficulties in treating π -conjugation effects. Journal of Chemical Physics, 2006, 124, 124112.	1.2	34

#	ARTICLE	IF	CITATIONS
2176	Better Understanding of the Ring-Cleavage Process of Cyanocyclopropyl Anionic Derivatives. A Theoretical Study Based on the Electron Localization Function. <i>Journal of Organic Chemistry</i> , 2006, 71, 754-762.	1.7	24
2177	How vitamin E scavenges DPPH radicals in polar protic media. <i>New Journal of Chemistry</i> , 2006, 30, 503.	1.4	96
2178	Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 364-382.	2.3	3,329
2179	N-Methylation Effects on the Coordination Chemistry of Cyclic Triamines with Divalent Transition Metals and Their Coll Dioxygen Carriers. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 304-314.	1.0	21
2180	Theoretical Studies of the Electronic Structure of Compounds of the Actinide Elements. , 2008, , 1893-2012.		31
2181	Cation- π Interactions and Oxidative Effects on Cu ⁺ and Cu ²⁺ Binding to Phe, Tyr, Trp, and His Amino Acids in the Gas Phase. Insights from First-Principles Calculations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24189-24199.	1.2	77
2182	A Density Functional That Accounts for Medium-Range Correlation Energies in Organic Chemistry. <i>Organic Letters</i> , 2006, 8, 5753-5755.	2.4	193
2183	Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12249-12258.	1.1	52
2184	Molecular Panels for Energy Transduction in C60-Based Conjugates. <i>Organic Letters</i> , 2006, 8, 2451-2454.	2.4	27
2185	Backbone Conformational Preferences and Pseudorotational Ring Puckering of 1-Aminocyclopentane-1-carboxylic Acid. <i>Journal of Physical Chemistry B</i> , 2006, 110, 21264-21271.	1.2	24
2186	Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. <i>Physical Review B</i> , 2006, 74, .	1.1	309
2187	First Principles Density Functional Study of the Adsorption and Dissociation of Carbonyl Compounds on Magnesium Oxide Nanosurfaces. <i>Journal of Physical Chemistry B</i> , 2006, 110, 25941-25949.	1.2	37
2188	Binding of Gold Clusters with DNA Base Pairs: A Density Functional Study of Neutral and Anionic GC ⁻ Aun and AT ⁻ Aun (n = 4, 8) Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7719-7727.	1.1	70
2189	Uniquely Strong Electronic Communication between [Mo ₂] Units Linked by Dioxolene Dianions. <i>Journal of the American Chemical Society</i> , 2006, 128, 3281-3290.	6.6	45
2190	First-principles calculations of the atomic and electronic structure of f-centers in the bulk and on the (001) surface of SrTiO ₃ . <i>Physical Review B</i> , 2006, 73, .	1.1	152
2191	Geometries and properties of excited states in the gas phase and in solution: Theory and application of a time-dependent density functional theory polarizable continuum model. <i>Journal of Chemical Physics</i> , 2006, 124, 094107.	1.2	1,143
2192	Induction of an Aromatic Six-Membered Nitrogen Ring via Cation- π Interaction. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12236-12240.	1.1	13
2193	Spectroscopic Studies of the Corrinoid/Iron-Sulfur Protein from <i>Moorella thermoacetica</i> . <i>Journal of the American Chemical Society</i> , 2006, 128, 5010-5020.	6.6	51

#	ARTICLE	IF	CITATIONS
2194	Target-Related Applications of First Principles Quantum Chemical Methods in Drug Design. <i>Chemical Reviews</i> , 2006, 106, 3497-3519.	23.0	109
2195	Gas-Phase Deprotonation of Uracil \sim Cu ²⁺ and Thiouracil \sim Cu ²⁺ Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1943-1950.	1.1	69
2196	On the accuracy of density functional theory in transition metal chemistry. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2006, 102, 203.	4.4	285
2197	Catalytic alcohol oxidation by an unsymmetrical 5-coordinate copper complex: electronic structure and mechanism. <i>Dalton Transactions</i> , 2006, , 159-167.	1.6	27
2198	Second-Harmonic Generation within theP212121Space Group, in a Series of Chiral (Salicylaldiminato)tin Schiff Base Complexes. <i>Chemistry of Materials</i> , 2006, 18, 1174-1183.	3.2	78
2199	Bond Length Alternation and Energy Band Gap of Polyyne. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9771-9774.	1.1	123
2200	Density Functional Theory and DFT+U Study of Transition Metal Porphines Adsorbed on Au(111) Surfaces and Effects of Applied Electric Fields. <i>Journal of the American Chemical Society</i> , 2006, 128, 3659-3668.	6.6	100
2201	Benchmark Study of DFT Functionals for Late-Transition-Metal Reactions \hat{e} . <i>Journal of Physical Chemistry A</i> , 2006, 110, 709-716.	1.1	223
2202	Density Functional Theory/Time-dependent DFT Studies on the Structures, Trend in DNA-binding Affinities, and Spectral Properties of Complexes [Ru(bpy) ₂ (p-R-pip)] ²⁺ (R = \hat{a} ^{\sim} OH, \hat{a} ^{\sim} CH ₃ , \hat{a} ^{\sim} H, \hat{a} ^{\sim} NO ₂). <i>Journal of Physical Chemistry A</i> , 2006, 110, 8174-8180.	1.1	52
2203	The Boat-Shaped Polyketide Resistoflavin Results from Re-Facial Central Hydroxylation of the Discoid Metabolite Resistomycin. <i>Journal of the American Chemical Society</i> , 2006, 128, 14619-14624.	6.6	40
2204	High electron affinities of bicyclo[n,n,0]perfluoroalkanes. <i>Molecular Physics</i> , 2006, 104, 1311-1324.	0.8	3
2205	Surface-Enhanced Resonance Raman Scattering and Density Functional Calculations of Hemicyanine Adsorbed on Colloidal Silver Surface. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1805-1811.	1.1	27
2206	Structure of RutileTiO ₂ (110) \hat{a} ^{\sim} (1 \hat{A} ^{\sim} 2): Formation ofTi ₂ O ₃ Quasi-1D Metallic Chains. <i>Physical Review Letters</i> , 2006, 96, 055502.	2.9	60
2207	Microhydration shell structure in Cl ₂ \hat{a} ^{\sim} TM \hat{a} ^{\sim} TMnH ₂ O clusters: A theoretical study. <i>Journal of Chemical Physics</i> , 2006, 125, 074309.	1.2	21
2208	Negative oxygen vacancies in HfO ₂ as charge traps in high-k stacks. <i>Applied Physics Letters</i> , 2006, 89, 082908.	1.5	295
2209	Quantum chemical study of the initial surface reactions of HfO ₂ atomic layer deposition on the hydroxylated GaAs(001)-4 \hat{A} ^{\sim} 2 surface. <i>Applied Physics Letters</i> , 2006, 89, 162905.	1.5	16
2210	SCRF-DFT and NMR Comparison of Tetracycline and 5a,6-Anhydrotetracycline in Solution. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24766-24774.	1.2	14
2211	Structure \hat{a} ^{\sim} Property Relationships in Push \hat{a} ^{\sim} Pull Amino/Cyanovinyl End-Capped Oligothiophenes: \hat{A} Quantum Chemical and Experimental Studies. <i>Journal of Organic Chemistry</i> , 2006, 71, 7509-7520.	1.7	81

#	ARTICLE	IF	CITATIONS
2212	Substituent Effect on a Family of Quinones in Aprotic Solvents: An Experimental and Theoretical Approach. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9411-9419.	1.1	69
2213	Interplay of Structure and Reactivity in a Most Unusual Furan Diels-Alder Reaction. <i>Journal of the American Chemical Society</i> , 2006, 128, 13130-13141.	6.6	46
2214	Metal-Metal Bonding in Mixed Valence Ni ²⁺ Complexes and Spectroscopic Evidence for a Ni ³⁺ Species. <i>Inorganic Chemistry</i> , 2006, 45, 4396-4406.	1.9	48
2215	Different types of biological proton transfer reactions studied by quantum chemical methods. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2006, 1757, 969-980.	0.5	56
2216	Conformational Isomerism of Electroactive Calix[4]arenes: Influence of the Electronic State in the Flexibility of Thiophene-Containing Calix[4]arene. <i>Journal of Organic Chemistry</i> , 2006, 71, 6952-6957.	1.7	14
2217	Ion Mobility Spectrometric Investigation of Aromatic Cations in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3514-3520.	1.1	27
2218	Octopolar Chromophores Based on Donor- and Acceptor-Substituted 1,3,5-Tris(phenylethynyl)benzenes: Impact of meta-Conjugation on the Molecular and Electronic Structure by Means of Spectroscopy and Theory. <i>Journal of Physical Chemistry B</i> , 2006, 110, 19198-19206.	1.2	31
2219	Combined Quantum Chemical Density Functional Theory and Spectroscopic Raman and UV-Vis-NIR Study of Oligothienoacenes with Five and Seven Rings. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5058-5065.	1.1	39
2220	Spectroscopic and Computational Studies of Reduction of the Metal versus the Tetrapyrrole Ring of Coenzyme F ₄₃₀ from Methyl-Coenzyme M Reductase. <i>Biochemistry</i> , 2006, 45, 11915-11933.	1.2	10
2221	Exploration of Ground and Excited Electronic States of Aromatic and Quinoid S,S-Dioxide Terthiophenes. Complementary Systems for Enhanced Electronic Organic Materials. <i>Journal of the American Chemical Society</i> , 2006, 128, 10134-10144.	6.6	55
2222	Quantum Chemical Study of Adsorption and Dissociation of H ₂ S on the Gallium-Rich GaAs (001)-4 Å ² Surface. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9529-9533.	1.2	9
2223	Reaction-Path Dynamics and Theoretical Rate Constants for the CH _n F _{4-n} + O ₃ + HOOO + CH _n -1F _{4-n} (n= 2,3) Reactions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11113-11119.	1.1	7
2224	Temperature and Pressure Dependence of the Rate Constants of the Reaction of NO ₃ Radical with CH ₃ SCH ₃ . <i>Journal of Physical Chemistry A</i> , 2006, 110, 7401-7405.	1.1	7
2225	Geometry and Solvent Dependence of the Electronic Spectra of the Amide Group and Consequences for Peptide Circular Dichroism. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4702-4711.	1.1	36
2226	Kinetic Study of the Gas-Phase Reaction of OH with Br ₂ . <i>Journal of Physical Chemistry A</i> , 2006, 110, 9169-9174.	1.1	12
2227	Autoxidative Activation of the Nematocide 1,3-Dichloropropene to Highly Genotoxic and Mutagenic Derivatives: A Consideration of Genotoxic/Carcinogenic Mechanisms. <i>Chemical Research in Toxicology</i> , 2006, 19, 952-959.	1.7	11
2228	Density Functional Calculations of ³ He Chemical Shift in Endohedral Helium Fullerenes: Neutral, Anionic, and Di-Helium Species. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12338-12341.	1.1	29
2229	Ancisheyne, the First N,C-Coupled Naphthylisoquinoline Alkaloid: Total Synthesis and Stereochemical Analysis. <i>Organic Letters</i> , 2006, 8, 1037-1040.	2.4	58

#	ARTICLE	IF	CITATIONS
2230	Strong Electronic Interaction between Two Dimolybdenum Units Linked by a Tetraazatetracene. <i>Inorganic Chemistry</i> , 2006, 45, 767-778.	1.9	30
2231	Chemistry Surrounding Monomeric Copper(I) Methyl, Phenyl, Anilido, Ethoxide, and Phenoxide Complexes Supported by N-Heterocyclic Carbene Ligands: A Reactivity Consistent with Both Early and Late Transition Metal Systems. <i>Inorganic Chemistry</i> , 2006, 45, 9032-9045.	1.9	91
2232	N- and P-Channel Transport Behavior in Thin Film Transistors Based on Tricyanovinyl-Capped Oligothiophenes. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14590-14597.	1.2	63
2233	Magnetic and Conductive Properties of Quinoidal Oligothiophenes. <i>Chemistry of Materials</i> , 2006, 18, 1539-1545.	3.2	32
2234	On the consequences of side chain flexibility and backbone conformation on hydration and proton dissociation in perfluorosulfonic acid membranes. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 2193.	1.3	109
2235	Substituent effect on the electrochemical behaviour of some ortho-substituted (aryl)(2-nitrobenzo[b]thiophen-3-yl)amines. A combined experimental and computational study. <i>Molecular Physics</i> , 2006, 104, 2961-2982.	0.8	8
2236	Reaction of C-Silylated $\hat{\iota}$ -Diazophosphines as Nucleophiles toward Carbonyl Compounds: A Mechanistic Study and Application to the Synthesis of Alkynes and $\hat{\iota}$ -Hydroxyphosphonamides. <i>Journal of Organic Chemistry</i> , 2006, 71, 5320-5327.	1.7	9
2237	Platinum Testbeds: Interaction with Oxygen. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11968-11974.	1.1	9
2238	High-Level ab Initio Studies of Hydrogen Abstraction from Prototype Hydrocarbon Systems. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11160-11173.	1.1	49
2239	Novel 5 $\hat{\iota}$ -Reductase Inhibitors: Synthesis, Structure-Activity Studies, and Pharmacokinetic Profile of Phenoxybenzoylphenyl Acetic Acids. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 748-759.	2.9	19
2240	Molecular Understanding of Alumina Supported Single-Site Catalysts by a Combination of Experiment and Theory. <i>Journal of the American Chemical Society</i> , 2006, 128, 9157-9169.	6.6	125
2241	Homogeneous Decomposition of Aryl- and Alkylimido Precursors for the Chemical Vapor Deposition of Tungsten Nitride: A Combined Density Functional Theory and Experimental Study. <i>Journal of the American Chemical Society</i> , 2006, 128, 13781-13788.	6.6	34
2242	Density Functional Study of Electron Paramagnetic Resonance Parameters and Spin Density Distributions of Dicopper(I) Complexes with Bridging Azo and Tetrazine Radical-Anion Ligands. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4021-4033.	1.1	18
2243	OH-Stretch Vibrational Spectroscopy of Hydroxymethyl Hydroperoxide. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7072-7079.	1.1	26
2244	Performance of the Effective Core Potentials of Ca, Hg, and Pb in Complexes with Ligands Containing N and O Donor Atoms. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1510-1519.	2.3	13
2245	About the choice of the protogenic group in polymer electrolyte membranes: Ab initio modelling of sulfonic acid, phosphonic acid, and imidazole functionalized alkanes. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4530.	1.3	203
2246	Direct Dynamics Study on Hydrogen Abstraction Reaction of CF ₃ CF ₂ CH ₂ OH with OH Radical. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5853-5859.	1.1	20
2247	Synthesis, X-ray, and DFT Study of the Double-Bond Pyramidalization in 1,7,8,9-Tetraphenyl-4,10,10-trimethyl-4-aza-10-silatricyclo[5.2.1.0.2,6]deca-8-ene-3,5-dione and Its Germanium Analogue. <i>Organometallics</i> , 2006, 25, 111-117.	1.1	6

#	ARTICLE	IF	CITATIONS
2248	Comprehensive Study of the Effects of Methylation on Tautomeric Equilibria of Nucleic Acid Bases. <i>Journal of Physical Chemistry B</i> , 2006, 110, 15564-15571.	1.2	21
2249	Theoretical and Experimental Studies of the Spin Trapping of Inorganic Radicals by 5,5-Dimethyl-1-PyrrolineN-Oxide (DMPO). 1. Carbon Dioxide Radical Anion. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13253-13258.	1.1	84
2250	Understanding the Selectivity in Hydrogenation of $\hat{1}\pm, \hat{1}^2$ -Unsaturated Aldehydes: A Water-Assisted Mechanism. <i>Organometallics</i> , 2006, 25, 854-861.	1.1	30
2251	Strong Electronic Communication by Direct Metal-Metal Interaction in Molecules with Halide-Bridged Dimolybdenum Pairs. <i>Inorganic Chemistry</i> , 2006, 45, 9493-9501.	1.9	18
2252	Evaluation of Effective Core Potentials and Basis Sets for the Prediction of the Geometries of Alkyltin Halides. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5893-5896.	1.1	27
2253	Spin-orbit splittings and energy band gaps calculated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. <i>Physical Review B</i> , 2006, 74, .	1.1	182
2254	Theoretical Insights, in the Liquid Phase, Into the Antioxidant Mechanism-Related Parameters in the 2-Monosubstituted Phenols. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11151-11159.	1.1	30
2255	Effects of Thioether Substituents on the O ₂ Reactivity of $\hat{1}^2$ -Diketiminato-Cu(I) Complexes: Probing the Role of the Methionine Ligand in Copper Monooxygenases. <i>Journal of the American Chemical Society</i> , 2006, 128, 3445-3458.	6.6	111
2256	EPR and ENDOR Study of Radiation-Induced Radical Formation in Purines: Sodium Inosine Crystals X-irradiated at 10 K. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6552-6562.	1.1	4
2257	Conformational Analysis of a Cyclopropane Analogue of Phenylalanine with Two Geminal Phenyl Substituents. <i>Journal of Physical Chemistry B</i> , 2006, 110, 5762-5766.	1.2	23
2258	Chemistry of 1,1,1,5,5,5-Hexafluoro-2,4-pentanedione on Si(100)-2 \times 1. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14337-14344.	1.2	18
2259	Structure and Stability of Salicylic Acid-Water Complexes and the Effect of Molecular Hydration on the Spectral Properties of Salicylic Acid. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5960-5964.	1.1	20
2260	Reaction Mechanisms and Kinetics for the Oxidations of Dimethyl Sulfide, Dimethyl Disulfide, and Methyl Mercaptan by the Nitrate Radical. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7682-7689.	1.1	11
2261	Thermodynamic Properties (Enthalpy, Bond Energy, Entropy, and Heat Capacity) and Internal Rotor Potentials of Vinyl Alcohol, Methyl Vinyl Ether, and Their Corresponding Radicals. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7925-7934.	1.1	88
2262	Dissolution Nature of Cesium Fluoride by Water Molecules. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3808-3815.	1.2	28
2263	Oxygen Atom Transfer Energetics: Assessment of the Effect of Method and Solvent. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4053-4056.	1.1	3
2264	Structures, Electron Affinities, and Harmonic Vibrational Frequencies of C ₆ H ₅ X/C ₆ H ₅ X-(X = N, S, NH). <i>Journal of Physical Chemistry A</i> , 2006, 110, 7682-7687.	1.1	6
2265	Selective Functionalization of the Si(100) Surface by a Bifunctional Alkynylamine Molecule: Density Functional Study of the Switching Adsorption Linkage. 2. <i>Journal of Physical Chemistry B</i> , 2006, 110, 7682-7687.	1.2	5

#	ARTICLE	IF	CITATIONS
2266	Quantifying Aromaticity at the Molecular and Supramolecular Limits: Comparing Homonuclear, Heteronuclear, and H-Bonded Systems. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 30-36.	2.3	54
2267	Characterizing the Potential Energy Surface of the Water Dimer with DFT: Failures of Some Popular Functionals for Hydrogen Bonding. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7268-7271.	1.1	48
2268	Combined In Situ EDXRD/EXAFS Investigation of the Crystal Growth of [Co(C ₆ H ₁₈ N ₄)] ₂ [Sb ₂ S ₄] under Solvothermal Conditions: Two Different Reaction Pathways Leading to the Same Product. <i>Chemistry of Materials</i> , 2006, 18, 1196-1205.	3.2	64
2269	Self-interaction-free exchange-correlation functional for thermochemistry and kinetics. <i>Journal of Chemical Physics</i> , 2006, 124, 091102.	1.2	179
2270	Anomalous Excited-State Dynamics of Lucifer Yellow CH in Solvents of High Polarity: Evidence for an Intramolecular Proton Transfer. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5585-5591.	1.1	24
2271	Transition from a Nonbonding to a Bonding Interaction in a Tetranuclear [Mo ₂] ₂ (μ_4 -OR) ₄ Cluster. <i>Inorganic Chemistry</i> , 2006, 45, 6387-6395.	1.9	14
2272	The Loss of Carbon Dioxide from Activated Perbenzoate Anions in the Gas Phase: Unimolecular Rearrangement via Epoxidation of the Benzene Ring. <i>Journal of Organic Chemistry</i> , 2006, 71, 7996-8005.	1.7	19
2273	Isopropylcyclopropane + OH Gas Phase Reaction: A Quantum Chemistry + CVT/SCT Approach. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1917-1924.	1.1	17
2274	Optical Excitations in Carbon Architectures Based on Dodecahydrotribenzo[18]annulene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1305-1318.	1.1	41
2275	A Combined Density Functional Theory and Coupled Cluster Method Investigation of the Structural Properties and Stabilities of Radical CH ₂ CP and Its Isomers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2411-2420.	1.1	1
2276	A Rare and Highly Oxidized Mo ^{25.5+} Unit Stabilized by Oxo Anions and Supported by Formamidinate Bridges. <i>Inorganic Chemistry</i> , 2006, 45, 9046-9052.	1.9	9
2277	Theoretical Study of NH ₃ Adsorption on Fe(110) and Fe(111) Surfaces. <i>Journal of Physical Chemistry B</i> , 2006, 110, 4846-4852.	1.2	69
2278	Direct Dynamics Study on the Reaction of N ₂ H ₄ with F Atom: A Hydrogen Abstraction Reaction?. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11636-11644.	1.1	6
2279	Electron Transfer in a Radical Ion Pair: Quantum Calculations of the Solvent Reorganization Energy. <i>Journal of Physical Chemistry B</i> , 2006, 110, 25115-25121.	1.2	13
2280	Insights into Photodissociation Dynamics of Propionyl Chloride from ab Initio Calculations and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2006, 110, 944-950.	1.1	11
2281	Aromaticity and Möbius Antiaromaticity in Monocyclic [11]Annulene Cations. <i>Journal of Organic Chemistry</i> , 2006, 71, 9271-9282.	1.7	23
2282	Lithium Cation as Radical-Polymerization Catalyst. <i>Journal of the American Chemical Society</i> , 2006, 128, 11278-11285.	6.6	23
2283	Photoexcitation of Dinucleoside Radical Cations: A Time-Dependent Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24181-24188.	1.2	45

#	ARTICLE	IF	CITATIONS
2284	On the Structure and Chemical Bonding of Tri-Tungsten Oxide Clusters W_3O_n - and W_3O_n ($n = 7-10$): W_3O_8 As A Potential Molecular Model for O-Deficient Defect Sites in Tungsten Oxides. <i>Journal of Physical Chemistry A</i> , 2006, 110, 85-92.	1.1	83
2285	Kinetics of the Hydrogen Abstraction $OH + Alkane \rightarrow H_2O + Alkyl$ Reaction Class: An Application of the Reaction Class Transition State Theory. <i>Journal of Physical Chemistry A</i> , 2006, 110, 473-484.	1.1	53
2286	Nickel Superoxide Dismutase Reaction Mechanism Studied by Hybrid Density Functional Methods. <i>Journal of the American Chemical Society</i> , 2006, 128, 7466-7475.	6.6	79
2287	Orbital Interactions in Fe(II)/Co(III) Heterobimetalloenes: Single versus Double Bridge. <i>Inorganic Chemistry</i> , 2006, 45, 2531-2542.	1.9	13
2288	Reactions of $F+(3P)$ and $F+(1D)$ with Silicon Oxide. Possibility of Spin-Forbidden Processes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7130-7137.	1.1	0
2289	Conformational Product Control in the Low-Temperature Photochemistry of Cyclopropylcarbenes. <i>Organic Letters</i> , 2006, 8, 4963-4966.	2.4	4
2290	Chemical Bonding in Sulfide Minerals. <i>Reviews in Mineralogy and Geochemistry</i> , 2006, 61, 231-264.	2.2	49
2291	Ab initio study of the nonlinear optical susceptibility of TeO_2 -based glasses. <i>Physical Review B</i> , 2006, 73, .	1.1	77
2292	Screened hybrid density functionals applied to solids. <i>Journal of Chemical Physics</i> , 2006, 124, 154709.	1.2	1,915
2293	Calculation of zero-field splitting parameters: Comparison of a two-component noncolinear spin-density-functional method and a one-component perturbational approach. <i>Journal of Chemical Physics</i> , 2006, 125, 054110.	1.2	66
2294	Electronic tuning of β^2 -diketiminate ligands with fluorinated substituents: effects on the O_2 -reactivity of mononuclear Cu(I) complexes. <i>Dalton Transactions</i> , 2006, , 4944-4953.	1.6	48
2295	Efficient Intermolecular $[2 + 2 + 2]$ Alkyne Cyclotrimerization in Aqueous Medium Using a Ruthenium(IV) Precatalyst. <i>Journal of the American Chemical Society</i> , 2006, 128, 15094-15095.	6.6	94
2296	Ester substitution in 2,2'-bithiophene: Analyses of the changes induced in the structural and electronic properties. <i>Synthetic Metals</i> , 2006, 156, 602-609.	2.1	9
2297	5. Chemical Bonding in Sulfide Minerals. , 2006, , 231-264.		2
2299	A Theoretical Elucidation of the Radical-Scavenging Power of Cyanidin. <i>Natural Product Communications</i> , 2006, 1, 1934578X0600100.	0.2	0
2300	Theoretical Study of the Diastereofacial Isomers of Aldrin and Dieldrin. <i>International Journal of Molecular Sciences</i> , 2006, 7, 35-46.	1.8	2
2301	Theoretical Study of Electronic Structures of [Peroxoporphinato]manganate $[Mn(P)(O_2)]^{3-}$ Anion. <i>Bulletin of the Chemical Society of Japan</i> , 2006, 79, 1201-1210.	2.0	5
2302	Theoretical Investigation of the Proton Affinity and Gas-Phase Basicity of Neutral x,y -Dihydroxybenzoic Acid and its Derivatives. <i>European Journal of Mass Spectrometry</i> , 2006, 12, 385-396.	0.5	7

#	ARTICLE	IF	CITATIONS
2303	Geometrical and electronic structures of the Sn_nCl and Sn_nCl_6^- ($n=1-6$) clusters. <i>Molecular Physics</i> , 2006, 104, 1861-1867.	0.8	6
2304	Electronic excitations in anti-aromatic dehydro[12]- and aromatic dehydro[18]annulenes: a time-dependent density functional theory study. <i>Molecular Physics</i> , 2006, 104, 933-941.	0.8	9
2305	Computational Molecular Basis for Improved Silica Surface Complexation Models. <i>Interface Science and Technology</i> , 2006, , 359-396.	1.6	9
2306	A qualitative study of amlodipine and its related compounds by electrospray ionization tandem mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2006, 20, 1715-1723.	0.7	10
2307	The fragmentation pathways of protonated Amiton in the gas phase: towards the structural characterisation of organophosphorus chemical warfare agents by electrospray ionisation tandem mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2006, 20, 1939-1948.	0.7	18
2308	Is combining meta-GGA correlation functionals with the OPTX exchange functional useful?. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 436-446.	1.0	11
2309	Gallium phosphides GAmPn ($m+n=2-5$) and their anions: Structures, electron affinities, and vibrational frequencies. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 968-980.	1.0	5
2310	Analysis of the bonding in $\text{XH}_3\text{X}'_2\text{Cu}^+$ ($\text{X}'=3/4\text{B, Al, Ga}$) complexes. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 659-663.	1.0	4
2311	Ab initio and DFT study of Y_3^+ hydration. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2236-2244.	1.0	8
2312	Kinetics and structural aspects of the cisplatin interactions with guanine: A quantum mechanical description. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2129-2144.	1.0	35
2313	On the stability of non-conventional π -complexes between Ni^+ and toluene, phenyl-silane and phenyl-germane. <i>Journal of Physical Organic Chemistry</i> , 2006, 19, 495-502.	0.9	3
2314	Three-dimensional model of the human aromatase enzyme and density functional parameterization of the iron-containing protoporphyrin IX for a molecular dynamics study of heme-cysteinato cytochromes. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 62, 1074-1087.	1.5	80
2315	Effect of hydrogen bonds on the energetics of macromolecules in the course of electron transfer. <i>Biophysics (Russian Federation)</i> , 2006, 51, 226-232.	0.2	5
2316	Photochemical transformations of 1,3,5-trioxane radical cations in freonic matrices at 77 K. <i>High Energy Chemistry</i> , 2006, 40, 259-266.	0.2	3
2317	Pyrene fluorescence quenching by aromatic azides. <i>Kinetics and Catalysis</i> , 2006, 47, 75-82.	0.3	7
2318	Correlation corrections based on the Schrödinger equation with a local potential. <i>Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)</i> , 2006, 100, 315-321.	0.2	1
2319	On the possibility of interpretation of the spectra of tetrapyrrole compounds and their radical ions on the basis of quantum-chemical calculations by the density functional method. <i>Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)</i> , 2006, 101, 862-870.	0.2	2
2320	Anion of hypericin is crucial to understanding the photosensitive features of the pigment. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 1414-1417.	1.0	40

#	ARTICLE	IF	CITATIONS
2321	A density functional theory study on the role of His-107 in arylamine N-acetyltransferase 2 acetylation. <i>Biophysical Chemistry</i> , 2006, 122, 215-220.	1.5	6
2322	State of hydrogen molecules confined in C60 fullerene and carbon nanocapsule structures. <i>Carbon</i> , 2006, 44, 397-406.	5.4	67
2323	A combined theoretical and experimental investigation about the influence of the dopant in the anodic electropolymerization of 1,4-tetrathiphene. <i>Chemical Physics</i> , 2006, 323, 407-412.	0.9	5
2324	Theoretical study on the Cl+CH3S(O)CH3 reaction. <i>Chemical Physics</i> , 2006, 324, 291-297.	0.9	1
2325	A theoretical study on the strength of two-center three-electron bonds in the NO3 radical adducts of reduced sulfur molecules, H2S, CH3SH, CH3SCH3, and CH3SSCH3. <i>Chemical Physics</i> , 2006, 324, 465-473.	0.9	13
2326	Free tetra- and hexa-coordinated platinum-cyanide dianions, and : A combined photodetachment photoelectron spectroscopic and theoretical study. <i>Chemical Physics</i> , 2006, 329, 230-238.	0.9	22
2327	Interpolation density values on a cartesian grid: Improving the efficiency of Lebedev based numerical integration in Kohn-Sham density functional algorithms. <i>Chemical Physics Letters</i> , 2006, 418, 490-495.	1.2	11
2328	Theoretical study of [XN6]2 ⁻ (X=O, S, Se, Te) systems. <i>Chemical Physics Letters</i> , 2006, 418, 272-280.	1.2	1
2329	Internal energy effects on charge stripping spectra of [C7H8] ⁺ and [C5H6] ⁺ radical cations. <i>Chemical Physics Letters</i> , 2006, 419, 139-143.	1.2	6
2330	Relationship between singlet-triplet excitation energies and the Kohn-Sham orbitals obtained with potentials that exhibit a wrong asymptotic behavior. <i>Chemical Physics Letters</i> , 2006, 419, 207-212.	1.2	12
2331	Theoretical evidence for the reaction of N-methyl-2-pyrrolidinone with carbon disulfide. <i>Chemical Physics Letters</i> , 2006, 420, 162-165.	1.2	9
2332	B3LYP, RHF and PM5 theoretical studies on phosphorescent cyclometalated Ir(III) complexes. <i>Chemical Physics Letters</i> , 2006, 420, 230-234.	1.2	5
2333	Non-growth ligand exchange reactions in atomic layer deposition of HfO2. <i>Chemical Physics Letters</i> , 2006, 421, 215-220.	1.2	23
2334	Theoretical study of activation CC double bond of C2H4 by Si^+ . <i>Chemical Physics Letters</i> , 2006, 421, 215-220.	1.2	12
2335	Electron affinities and ionization potentials of 4d and 5d transition metal atoms by CCSD(T), MP2 and density functional theory. <i>Chemical Physics Letters</i> , 2006, 423, 81-86.	1.2	21
2336	Synthesis, X-ray, spectroelectrochemical, and theoretical studies of a tricyanovinyl-capped quaterthiophene: A correlation of semiconductor performance with physical properties. <i>Chemical Physics Letters</i> , 2006, 425, 251-256.	1.2	6
2337	Coexistence of metastable nitric acid dihydrates: A molecular level contribution to understanding the formation of polar stratospheric clouds crystals. <i>Chemical Physics Letters</i> , 2006, 426, 20-25.	1.2	7
2338	Theoretical study of activation CO bond of CH3OCH3 by Ti ⁺ in the gas phase. <i>Chemical Physics Letters</i> , 2006, 427, 271-275.	1.2	13

#	ARTICLE	IF	CITATIONS
2339	Identification of the intrinsic conformational properties of 1-aminocyclobutane-1-carboxylic acid. <i>Chemical Physics Letters</i> , 2006, 429, 558-562.	1.2	16
2340	The oxidation pathways of Ti ⁺ by acetaldehyde in the gas phase: A density functional theory investigation. <i>Chemical Physics Letters</i> , 2006, 431, 56-61.	1.2	16
2341	A series of novel aromatic compounds with a planar N ₆ ring. <i>Chemical Physics Letters</i> , 2006, 432, 331-335.	1.2	15
2342	Theoretical studies on the reactions X+CHBrF ₂ (X=F, Br). <i>Chemical Physics Letters</i> , 2006, 432, 6-10.	1.2	1
2343	Theoretical survey of the potential energy surface of Ni ⁺⁺ acetone reaction. <i>Chemical Physics Letters</i> , 2006, 432, 27-32.	1.2	22
2344	A B3LYP study of proton transfer path within a complex of benzene radical cation and water cluster. <i>Chemical Physics Letters</i> , 2006, 432, 22-26.	1.2	5
2345	On the active site for hydrolysis of aryl amides and choline esters by human cholinesterases. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 4586-4599.	1.4	41
2346	Synthetic and theoretical study on proline-catalyzed Knoevenagel condensation in ionic liquid. <i>Journal of Molecular Catalysis A</i> , 2006, 253, 212-221.	4.8	68
2347	Conformational isomerism and phase transitions in tetraethylammonium bis(trifluoromethanesulfonyl)imide Et ₄ N ⁺ TFSI. <i>Journal of Molecular Structure</i> , 2006, 783, 145-156.	1.8	79
2348	¹ H NMR and DFT studies of steric effects on intermolecular C-H...O hydrogen bonding in solution. <i>Journal of Molecular Structure</i> , 2006, 789, 43-51.	1.8	8
2349	Cu ⁺ association to some Ph-X (X=OH, NH ₂ , CHO, COOH, CF ₃) phenyl derivatives.. <i>International Journal of Mass Spectrometry</i> , 2006, 255-256, 20-27.	0.7	27
2350	Unimolecular reactions of halogeno phenylarsenium ions: Kinetic energy release during the elimination of halogen hydride. <i>International Journal of Mass Spectrometry</i> , 2006, 249-250, 130-137.	0.7	4
2351	Dynamics of chemical and charge transfer reactions of molecular dications: VI. <i>International Journal of Mass Spectrometry</i> , 2006, 255-256, 150-163.	0.7	11
2352	Synthesis, characterization and nonlinear optical properties in a series of new chiral organotin(IV) Schiff base complexes. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 1722-1732.	0.8	51
2353	The mechanism of transition metal catalyzed carbonylation of allyl halides: A theoretical investigation. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4498-4507.	0.8	9
2354	FTIR, FT-Raman spectra and ab initio DFT vibrational analysis of 2-amino-5-chloropyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 64, 586-594.	2.0	39
2355	Electron capture dissociation of peptides metalated with alkaline-earth metal ions. <i>Journal of the American Society for Mass Spectrometry</i> , 2006, 17, 757-771.	1.2	54
2356	Ab initio and DFT investigation of fluorinated methyl hydroperoxides: Structures, rotational barriers, and thermochemical properties. <i>Journal of Fluorine Chemistry</i> , 2006, 127, 54-62.	0.9	11

#	ARTICLE	IF	CITATIONS
2357	Radical trifluoromethylation of Ti ate enolate: possible intervention of transformation of Ti(IV) to Ti(III) for radical termination. <i>Journal of Fluorine Chemistry</i> , 2006, 127, 539-544.	0.9	43
2358	Synthesis, characterization and DNA-binding of novel chiral complexes λ^2 - and λ^1 -[Ru(bpy)2L]2+ (L=o-mopip) <i>Tj ETQq1,1 0.784314 rgB</i>	1.5	146
2359	Theoretical studies of enzyme mechanisms involving high-valent iron intermediates. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 727-743.	1.5	48
2360	DRIFTS evidence for the formation of binuclear Cu(I) dinitrogen complexes upon adsorption of N2 on CuZSM-5. <i>Microporous and Mesoporous Materials</i> , 2006, 94, 320-324.	2.2	26
2361	Muoniated acyl and thioacyl radicals. <i>Physica B: Condensed Matter</i> , 2006, 374-375, 299-302.	1.3	7
2362	The effects of backbone conformation on hydration and proton transfer in the α -short-side-chain TM perfluorosulfonic acid membrane. <i>Solid State Ionics</i> , 2006, 177, 2385-2390.	1.3	78
2363	DFT study on dissociative adsorption of SiH4 and GeH4 on SiGe(100)-2 \times 1 surface. <i>Surface Science</i> , 2006, 600, 3194-3201.	0.8	9
2364	Chiral discrimination of ibuprofen isomers in β -cyclodextrin inclusion complexes: experimental (NMR) and theoretical (MD, MM/GBSA) studies. <i>Tetrahedron</i> , 2006, 62, 4162-4172.	1.0	46
2365	Rh-catalyzed alkene oxidation: a highly efficient and selective process for preparing N-alkoxysulfonyl aziridines. <i>Tetrahedron</i> , 2006, 62, 11331-11342.	1.0	122
2366	Synthesis and conformational analysis of naphth[1 α :2,2 α :5,6][1,3]oxazino[3,2-c][1,3]benzoxazine and naphth[1 α :2,2 α :5,6][1,3]oxazino[3,4-c][1,3]benzoxazine derivatives. <i>Tetrahedron</i> , 2006, 62, 11081-11089.	1.0	70
2367	The first total synthesis of (R)-convolutamydine A. <i>Tetrahedron</i> , 2006, 62, 12017-12024.	1.0	117
2368	Theoretical study of the bifunctional-urea catalyzed Michael reaction of 1,3-dicarbonyl compounds and nitroolefins: reaction mechanism and enantioselectivity. <i>Tetrahedron: Asymmetry</i> , 2006, 17, 1611-1616.	1.8	37
2369	Chemoenzymatic synthesis of enantiomerically pure tricyclic benzomorphan analogues. <i>Tetrahedron: Asymmetry</i> , 2006, 17, 3046-3050.	1.8	10
2370	Synthesis of 2H-pyrroles via the 1,3-dipolar cycloaddition reaction of nitrile ylides with acrylamides. <i>Tetrahedron Letters</i> , 2006, 47, 477-481.	0.7	14
2371	Density functional study of propylene oxidation on Ag and Au surfaces. Comparison to ethylene oxidation. <i>Computational and Theoretical Chemistry</i> , 2006, 762, 57-67.	1.5	11
2372	The phosphorus clusters Pn (n=1-6) and their anions: Structures and electron affinities. <i>Computational and Theoretical Chemistry</i> , 2006, 759, 225-238.	1.5	30
2373	Structure, stability and chemical bonding character of covalent boron azides BX(N3)2 (X=F, Cl, Br). <i>Computational and Theoretical Chemistry</i> , 2006, 759, 171-176.	1.5	0
2374	Theoretical study of the gas-phase acidity and aromaticity of a novel derivative of nitrogen squaric acid. <i>Computational and Theoretical Chemistry</i> , 2006, 763, 181-186.	1.5	11

#	ARTICLE	IF	CITATIONS
2375	Theoretical study on structures and energetics of Ge ₂ P ₂ . Computational and Theoretical Chemistry, 2006, 764, 47-52.	1.5	3
2376	Density functional study of noncovalent catalysis of the Diels-Alder reaction by the neutral hydrogen bond donors thiourea and urea. Computational and Theoretical Chemistry, 2006, 765, 45-52.	1.5	15
2377	A theoretical treatment of the intersystem crossing in the spin-forbidden reaction. Computational and Theoretical Chemistry, 2006, 770, 1-6.	1.5	1
2378	Thiol-thione tautomerism in 2-pyridinethione: Effect of hydration. Computational and Theoretical Chemistry, 2006, 767, 51-60.	1.5	19
2379	Bonding and solvation preferences of nickel complexes [Ni(S ₂ PR ₂) ₂] (R=H, Me, OMe) according a natural bond orbital analysis. Computational and Theoretical Chemistry, 2006, 767, 37-41.	1.5	13
2380	Combined computational and crystallographic study of the oxidised states of [NiFe] hydrogenase. Computational and Theoretical Chemistry, 2006, 770, 199-219.	1.5	52
2381	Theoretical study of group transfer from multiply-bonded nickel complexes to ethylene. Computational and Theoretical Chemistry, 2006, 801, 47-53.	1.5	15
2382	Dienamine Catalysis: Organocatalytic Asymmetric β -Amination of α,β -Unsaturated Aldehydes. Journal of the American Chemical Society, 2006, 128, 12973-12980.	6.6	380
2383	Crossed-beam radical-radical reaction dynamics of O(P ₃)+C ₃ H ₃ ⁺ H(S ₂)+C ₃ H ₂ O. Journal of Chemical Physics, 2006, 124, 204320.	1.2	20
2384	Atomistic Models of OH Defects in Nominally Anhydrous Minerals. Reviews in Mineralogy and Geochemistry, 2006, 62, 67-83.	2.2	23
2385	Heterolytic Splitting of H ₂ and CH ₄ on γ -Alumina as a Structural Probe for Defect Sites. Journal of Physical Chemistry B, 2006, 110, 23944-23950.	1.2	141
2386	The Guanine Cation Radical: Investigation of Deprotonation States by ESR and DFT. Journal of Physical Chemistry B, 2006, 110, 24171-24180.	1.2	133
2387	Single-Electron Oxidation of Monomeric Copper(I) Alkyl Complexes: Evidence for Reductive Elimination through Bimolecular Formation of Alkanes. Organometallics, 2006, 25, 4097-4104.	1.1	42
2388	The molecular and electronic structure of the Mo ₁₂ S ₄ macromolecule as a model of the active component of a hydrodesulfurization catalyst. Russian Journal of Physical Chemistry A, 2006, 80, 1083-1087.	0.1	2
2389	The molecular mechanism of low-temperature decomposition of hydrogen sulfide under conjugated chemisorption-catalysis conditions. Russian Journal of Physical Chemistry A, 2006, 80, 1403-1410.	0.1	18
2390	Quinone-sensitized Steady-state Photolysis of Acetophenone Oximes Under Aerobic Conditions: Kinetics and Product Studies. Photochemistry and Photobiology, 2006, 82, 110.	1.3	14
2391	A Theoretical Elucidation on the Solvent-dependent Photosensitive Behaviors of C ₆₀ . Photochemistry and Photobiology, 2006, 82, 798.	1.3	30
2392	Molecular orientation dependence of ortho-para H ₂ conversion on Fe(OH) ₃ cluster induced by hyperfine contact interaction. European Physical Journal D, 2006, 38, 99-101.	0.6	4

#	ARTICLE	IF	CITATIONS
2393	Ab initio study for structure, electric properties and light emission of linear-trans-quinacridone. <i>European Physical Journal D</i> , 2006, 38, 199-201.	0.6	1
2394	Theoretical study of the molecular properties of benzyl azide, 2-, 3- and 4-methyl benzyl azide. <i>European Physical Journal D</i> , 2006, 39, 379-384.	0.6	8
2395	Semiempirical hybrid density functional with perturbative second-order correlation. <i>Journal of Chemical Physics</i> , 2006, 124, 034108.	1.2	2,729
2396	Mechanism of a Soluble Fumarate Reductase from <i>Shewanella frigidimarina</i> : A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 10550-10556.	1.2	5
2397	Density functional study of the l-proline-catalyzed α -aminooxylation of aldehydes reaction: The reaction mechanism and selectivity. <i>Structural Chemistry</i> , 2006, 17, 97-104.	1.0	15
2398	Experimental and DFT Studies on the DNA-binding Properties of Ruthenium(II) Complexes [Ru(phen) ₂ L] ²⁺ (L = o-MOP, o-MP, o-CP and o-NP). <i>Transition Metal Chemistry</i> , 2006, 31, 277-285.	0.7	6
2399	DFT study of the structural characteristics of the yttrium(3+) aqua ion. <i>Journal of Structural Chemistry</i> , 2006, 47, 413-419.	0.3	9
2400	A DFT Study of Hydrogen-deuterium Exchange over Oxidized and Reduced Gallium Species in Ga/HZSM-5 Zeolite. <i>Catalysis Letters</i> , 2006, 108, 187-191.	1.4	12
2401	Models for dioxygen activation by the CuB site of dopamine α -monooxygenase and peptidylglycine α -hydroxylating monooxygenase. <i>Journal of Biological Inorganic Chemistry</i> , 2006, 11, 197-205.	1.1	44
2402	Theoretical study of [XN ₅] ⁻ (X=O, S, Se, Te) systems. <i>Journal of Molecular Modeling</i> , 2006, 12, 805-811.	1.8	4
2403	The Arrangement of First- and Second-shell Water Molecules Around Metal Ions: Effects of Charge and Size. <i>Theoretical Chemistry Accounts</i> , 2006, 115, 100-112.	0.5	78
2404	Ab initio studies of small Al _m Fe _n clusters. <i>Theoretical Chemistry Accounts</i> , 2006, 115, 32-36.	0.5	7
2405	Electronic Structures of 5d Transition Metal Monoxides by Density Functional Theory. <i>Theoretical Chemistry Accounts</i> , 2006, 117, 115-122.	0.5	49
2406	Molecular view of copper deposition chemistry: (Hexafluoroacetylacetonate)Cu(vinyltrimethylsilane) on a Si(100)-2 \times 1 surface. <i>Surface Science</i> , 2006, 600, 3313-3320.	0.8	24
2407	Ortho-para H ₂ conversion on multiple-decked sandwich clusters of M(C ₆ H ₆) ₂ (M=Mn, Fe, Co) induced by an inhomogeneity of spin density distribution. <i>Thin Solid Films</i> , 2006, 509, 223-226.	0.8	7
2408	Proton dissociation is important to understanding structure-activity relationships of gallic acid antioxidants. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 4095-4098.	1.0	59
2409	Effects of oxygenates and moisture on adsorptive desulfurization of liquid fuels with Cu(I)Y zeolite. <i>Catalysis Today</i> , 2006, 116, 512-518.	2.2	44
2410	Comprehensive DFT and MO studies on glyoxalic acid oxime and related ions in gas phase and solution: Conformations, basicities and acidities. <i>Chemical Physics</i> , 2006, 321, 311-324.	0.9	12

#	ARTICLE	IF	CITATIONS
2411	Theoretical investigation of the coexistence of $\hat{1}\pi$ and $\hat{1}^2$ -nitric acid trihydrates (NAT) molecular conformations. <i>Chemical Physics</i> , 2006, 324, 210-215.	0.9	8
2412	Theoretical study of adducts of dimethyl sulfide with hydroperoxyl and hydroxyl radicals. <i>Chemical Physics</i> , 2006, 326, 335-343.	0.9	11
2413	Misleading aspects of the viscosity effect on the heterogeneous electron transfer reactions. <i>Chemical Physics</i> , 2006, 326, 123-137.	0.9	10
2414	Avoiding self-repulsion in density functional description of biased molecular junctions. <i>Chemical Physics</i> , 2006, 329, 266-275.	0.9	31
2415	Characterization of synthetic oxomanganese complexes and the inorganic core of the O ₂ -evolving complex in photosystem II: Evaluation of the DFT/B3LYP level of theory. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 786-800.	1.5	99
2416	A comprehensive density functional theory study of ethane dehydrogenation over reduced extra-framework gallium species in ZSM-5 zeolite. <i>Journal of Catalysis</i> , 2006, 240, 73-84.	3.1	99
2417	Fine Tuning of the Electronic Properties of Linear π -Conjugated Oligomers by Covalent Bridging. <i>Chemistry - A European Journal</i> , 2006, 12, 1244-1255.	1.7	33
2418	A Stacking Interaction between a Bridging Hydrogen Atom and Aromatic π Density in then-B18H22 ²⁺ Benzene System. <i>Chemistry - A European Journal</i> , 2006, 12, 2571-2578.	1.7	26
2419	Tuning of Electronic Properties in Thienyl-Phosphole π -Conjugated Systems through P-Functionalization Monitored by Raman Spectroscopy. <i>Chemistry - A European Journal</i> , 2006, 12, 3759-3767.	1.7	26
2420	Optical, Redox, and NLO Properties of Tricyanovinyl Oligothiophenes: Comparisons between Symmetric and Asymmetric Substitution Patterns. <i>Chemistry - A European Journal</i> , 2006, 12, 5458-5470.	1.7	37
2421	Density Functional Studies on the Nazarov Reaction Involving Cyclic Systems. <i>Chemistry - A European Journal</i> , 2006, 12, 2836-2845.	1.7	42
2422	A QM/MM Study of Cisplatin ²⁺ -DNA Oligonucleotides: From Simple Models to Realistic Systems. <i>Chemistry - A European Journal</i> , 2006, 12, 5747-5756.	1.7	60
2423	An Experimental and Theoretical Investigation of Gas-Phase Reactions of Ca ²⁺ with Glycine. <i>Chemistry - A European Journal</i> , 2006, 12, 6787-6796.	1.7	57
2424	Gas-Phase Protonation and Deprotonation of Acrylonitrile Derivatives Ni $\frac{1}{2}$ Ci $\frac{1}{2}$ CHi $\frac{3}{4}$ CHi $\frac{1}{4}$ X (X=CH ₃ , NH ₂), Tj ETQq 1 1 0.784314 r g B	1.7	17
2425	Understanding Sulfone Behavior in Palladium-Catalyzed Domino Reactions with Aryl Iodides. <i>Chemistry - A European Journal</i> , 2006, 12, 4576-4583.	1.7	18
2426	Experimental and Theoretical Characterization of Superoxide Complexes [W ₂ O ₆ (O ₂ ⁻)] and [W ₃ O ₉ (O ₂ ⁻)]: Models for the Interaction of O ₂ with Reduced W Sites on Tungsten Oxide Surfaces. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 657-660.	7.2	66
2427	Precedent and Theory Unite in the Hypothesis of a Highly Selective Fluoride Receptor. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 2890-2893.	7.2	111
2428	Seemingly Simple Stereoelectronic Effects in Alkane Isomers and the Implications for Kohn ²⁺ -Sham Density Functional Theory. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 4460-4464.	7.2	360

#	ARTICLE	IF	CITATIONS
2429	Fixation of CO ₂ by Magnesium Cations: A Reinterpretation. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 5331-5334.	7.2	21
2430	Spectroscopic Comparison of Dinuclear Ti ⁺ and Ti ²⁺ 1/4-1:1:1 Dinitrogen Complexes with Cp*/Pentafulvene and Amine/Amide Ligation: Moderate versus Strong Activation of N ₂ . <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 291-297.	1.0	22
2431	The UV/Vis Spectrum of Potassium Heptacyanovanadate(III): A Theoretical Multi-Reference Configuration Interaction Study Combined with Low-Temperature Experiments. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 1588-1593.	1.0	3
2432	Kinetic and Thermodynamic Aspects of the CT and T-Shaped Adduct Formation Between 1,3-Dimethylimidazoline-2-thione (or -2-selone) and Halogens. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 2166-2174.	1.0	19
2433	Affinity of Polypyridines Towards CdII and CoII Ions: a Thermodynamic and DFT Study. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 3738-3745.	1.0	24
2434	Chromogenic Meroterpenoids from the Mushrooms <i>Russula ochroleuca</i> and <i>R. viscida</i> . <i>European Journal of Organic Chemistry</i> , 2006, 2006, 1023-1033.	1.2	52
2435	The Mechanism of Semibullvalene Bromination. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 738-745.	1.2	7
2436	Simultaneous Regio- and Enantiodifferentiation in Carbohydrate Coupling. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 3947-3959.	1.2	13
2437	Study of the Substituent-Influenced Anomeric Effect in the Ring-Chain Tautomerism of 1-Alkyl-3-aryl-naphth[1,2-e][1,3]oxazines. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 4670-4675.	1.2	8
2438	Electronic structures of 3d-metal mononitrides. <i>Journal of Computational Chemistry</i> , 2006, 27, 267-276.	1.5	12
2439	Hybrid density functional theory for π -stacking interactions: Application to benzenes, pyridines, and DNA bases. <i>Journal of Computational Chemistry</i> , 2006, 27, 491-504.	1.5	236
2440	Quantum chemistry applied to the mechanisms of transition metal containing enzymes—Cytochrome c oxidase, a particularly challenging case. <i>Journal of Computational Chemistry</i> , 2006, 27, 1373-1384.	1.5	66
2441	Characterization of the structure and reactivity of monocopper-oxygen complexes supported by β -diketiminato and anilido-imine ligands. <i>Journal of Computational Chemistry</i> , 2006, 27, 1950-1961.	1.5	54
2442	Substituent Effect on Proton Affinity of Imidazole in Cu,Zn-Superoxide Dismutase. <i>Chinese Journal of Chemistry</i> , 2006, 24, 822-824.	2.6	2
2443	What a Role did Histidine Residue Play in Arylamine N-Acetyltransferase 2 Acetylation? A Quantum Chemistry Study. <i>Chinese Journal of Chemistry</i> , 2006, 24, 1279-1281.	2.6	0
2444	Rational Design of Aziridine-Containing Cysteine Protease Inhibitors with Improved Potency: Studies on Inhibition Mechanism. <i>ChemMedChem</i> , 2006, 1, 1021-1028.	1.6	39
2445	Computational Study of ¹⁹ F NMR Spectra of Double Four Ring-Containing Si/Ge-Zeolites. <i>ChemPhysChem</i> , 2006, 7, 1092-1099.	1.0	46
2446	Theoretical Investigation of the Decarbonylation of Acetaldehyde by Fe ⁺ and Cr ⁺ . <i>ChemPhysChem</i> , 2006, 7, 1345-1354.	1.0	27

#	ARTICLE	IF	CITATIONS
2447	The Conformations of Alkanes Adsorbed on Zeolitic Cations. <i>ChemPhysChem</i> , 2006, 7, 1657-1660.	1.0	39
2448	A Theoretical Investigation of the Gas-Phase Oxidation Reaction of the Saturated tert-Butyl Radical. <i>ChemPhysChem</i> , 2006, 7, 2526-2532.	1.0	10
2449	(π - π)-double aromatic and π - σ -mixed aromatic boron compounds with two electrons delocalized over three centers. <i>Heteroatom Chemistry</i> , 2006, 17, 224-237.	0.4	44
2450	Eremophilane esters of <i>Robinsonia gerberifolia</i> and their rearranged products. Study of the coupling constants $^2J_{\text{H}}$, $^3J_{\text{H}}$, $^4J_{\text{H}}$. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 30-34.	1.1	3
2451	Collision-induced dissociation studies of protonated ether $(\text{H}_2\text{O})_n$ ($n = 1-3$) clusters. <i>Journal of Mass Spectrometry</i> , 2006, 41, 242-247.	0.7	4
2452	Carbon-rich Compounds: Computational Considerations. , 2006, , 334-382.		0
2457	Magnetic Properties of Quinoidal Oligothiophenes: More Than Good Candidates for Ambipolar Organic Semiconductors?. <i>Advanced Functional Materials</i> , 2006, 16, 531-536.	7.8	42
2458	Electronic Structure Calculations for Nanomolecular Systems. , 2006, , 77-116.		3
2459	Quantum chemical study of the initial surface reactions in atomic layer deposition of TiN on the SiO ₂ surface. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 5937-5944.	0.7	4
2460	Application of Wigner and Husimi intracule based electron correlation models to excited states. <i>Journal of Chemical Physics</i> , 2006, 125, 074104.	1.2	10
2461	Intensity enhancement of the vibrational spectrum of oxygen when attached to a platinum nanocluster. <i>Journal of Chemical Physics</i> , 2006, 125, 174302.	1.2	1
2462	H^2D isotope effect on porphine and porphycene molecules with multicomponent hybrid density functional theory. <i>Journal of Chemical Physics</i> , 2006, 125, 244105.	1.2	72
2463	Structural implications of ring shape, dimension, and metal atom insertion in nanosized cyclic oligothiophenes: Joint Raman and density functional theory study. <i>Journal of Chemical Physics</i> , 2006, 125, 044518.	1.2	12
2464	Hybrid exchange-correlation functional for core, valence, and Rydberg excitations: Core-valence-Rydberg B3LYP. <i>Journal of Chemical Physics</i> , 2006, 125, 064109.	1.2	65
2465	The role of the ring nitrogen and the amino group in the solvent dependence of the excited-state dynamics of 3-aminoquinoline. <i>Journal of Chemical Physics</i> , 2006, 125, 054513.	1.2	45
2466	Search for suitable approximation methods for fullerene structure and relative stability studies: Case study with C ₅₀ . <i>Journal of Chemical Physics</i> , 2006, 125, 094105.	1.2	19
2467	Density functional theory of complex transition densities. <i>Journal of Chemical Physics</i> , 2006, 125, 124104.	1.2	27
2468	Electronically excited states of tryptamine and its microhydrated complex. <i>Journal of Chemical Physics</i> , 2006, 125, 124309.	1.2	27

#	ARTICLE	IF	CITATIONS
2469	Combined experimental-theoretical study of the lower excited singlet states of paravinyl phenol, an analog of the paracoumaric acid chromophore. Journal of Chemical Physics, 2006, 125, 204303.	1.2	14
2470	Addition of hydrogen atom/hydride anion to the double bonds of cytosine tautomers: radical and anion structures and energetics. Molecular Physics, 2006, 104, 2347-2366.	0.8	7
2471	Dipole moments from atomic-number-dependent potentials in analytic density-functional theory. Journal of Chemical Physics, 2006, 125, 214104.	1.2	3
2472	Benchmarking the performance of density functional theory based Green's function formalism utilizing different self-energy models in calculating electronic transmission through molecular systems. Journal of Chemical Physics, 2006, 125, 204717.	1.2	27
2473	A restricted-open-shell complete-basis-set model chemistry. Journal of Chemical Physics, 2006, 125, 094106.	1.2	208
2474	A theoretical study of the chiroptical properties of molecules with isotopically engendered chirality. Journal of Chemical Physics, 2006, 124, 174301.	1.2	52
2475	A comparative ab initio study of Br ₂ and Br ₂ water clusters. Journal of Chemical Physics, 2006, 124, 024322.	1.2	34
2476	Adsorption at Adsorption Sites: Halogen Atoms on Alkali Halide Surfaces. Physical Review Letters, 2006, 97, 046802.	2.9	10
2477	Stabilization mechanism of Si ₁₂ cage clusters by encapsulation of a transition-metal atom: A density-functional theory study. Physical Review B, 2006, 74, .	1.1	60
2478	Exchange energy gradients with respect to atomic positions and cell parameters within the Hartree-Fock $\hat{\Gamma}$ -point approximation. Journal of Chemical Physics, 2006, 124, 214105.	1.2	3
2479	The electronic structure of oxo-Mn(salen): Single-reference and multireference approaches. Journal of Chemical Physics, 2006, 124, 144314.	1.2	43
2480	Spin-dependent electronic transport through a porphyrin ring ligating an Fe(II) atom: An ab initio study. Physical Review B, 2006, 74, .	1.1	41
2481	Frequency-dependent nonlinear optical properties of CdSe clusters. Physical Review B, 2006, 74, .	1.1	32
2482	Explicit role of dynamical and nondynamical electron correlations on broken symmetry in C ₄ N ₂ clusters. Physical Review B, 2006, 73, .	1.1	13
2483	Time-dependent density functional theory calculations for core-excited states: Assessment of standard exchange-correlation functionals and development of a novel hybrid functional. Journal of Chemical Physics, 2006, 124, 094105.	1.2	73
2484	Energy gradients with respect to atomic positions and cell parameters for the Kohn-Sham density-functional theory at the $\hat{\Gamma}$ point. Journal of Chemical Physics, 2006, 124, 224107.	1.2	2
2485	Axially Chiral Directly $\hat{\Gamma}^2$ -Linked Bisporphyrins: Synthesis and Stereostructure. Organic Letters, 2006, 8, 4743-4746.	2.4	60
2486	Direct Experimental Probe of the On-Site Coulomb Repulsion in the Doubly Charged Fullerene Anion C ₇₀ ²⁻ . Physical Review Letters, 2006, 96, 143002.	2.9	71

#	ARTICLE	IF	CITATIONS
2487	Density functional study of CrCl_2 : Structural, electronic, and magnetic properties. <i>Physical Review B</i> , 2006, 74, .	1.1	14
2488	First-Principles Calculations for Chemical Reaction between Sodium Diethyldithiocarbamate and Transition-Metal (Cr) atom to Produce $\text{Cr}(\text{DDC})_3$ and $\text{Cr}(\text{DDC})_2\text{ODDC}$. <i>Japanese Journal of Applied Physics</i> , 2006, 45, L1103-L1105.	0.8	3
2489	Direct dynamics study on the hydrogen abstraction reactions $\text{N}_2\text{H}_4 + \text{R}^\ddagger \rightarrow \text{N}_2\text{H}_3 + \text{RH}$ ($\text{R} = \text{NH}_2, \text{CH}_3$). <i>Journal of Chemical Physics</i> , 2006, 125, 064304.	1.2	10
2490	Orbital-dependent nonlocal correlation energy functional constructed from a Jastrow function: Application to atoms and ions. <i>Physical Review A</i> , 2006, 73, .	1.0	3
2491	From local hybrid functionals to ϵ -localized local hybrid potentials: Formalism and thermochemical tests. <i>Journal of Chemical Physics</i> , 2006, 124, 204102.	1.2	64
2492	Analysis of the vibrational spectra of chiral liquid crystalline thioesters. <i>Liquid Crystals</i> , 2006, 33, 219-225.	0.9	4
2493	Mechanism for the dissolution of olivine series minerals in acidic solutions. <i>American Mineralogist</i> , 2006, 91, 455-458.	0.9	50
2494	Spectroscopic characterization of the ground and low-lying electronic states of GaN via anion photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , 2006, 124, 064303.	1.2	21
2495	QSAR AND ACTION MECHANISM OF TROXACITABINE PRODRUGS WITH ANTITUMOR ACTIVITY. <i>Journal of Theoretical and Computational Chemistry</i> , 2007, 06, 947-958.	1.8	7
2496	Efficient evaluation of analytic vibrational frequencies in Hartree-Fock and density functional theory for periodic nonconducting systems. <i>Journal of Chemical Physics</i> , 2007, 127, 144106.	1.2	28
2497	Modeling and Characterization of Nitrogen-Enhanced Negative-Bias Temperature Instability in p-Channel MOSFETs. <i>Journal of the Electrochemical Society</i> , 2007, 154, G255.	1.3	5
2498	A thermochemically competitive local hybrid functional without gradient corrections. <i>Journal of Chemical Physics</i> , 2007, 126, 011103.	1.2	113
2499	QSAR AND MOLECULAR DESIGN OF BENZO[B]ACRONYCINE DERIVATIVES AS ANTITUMOR AGENTS. <i>Journal of Theoretical and Computational Chemistry</i> , 2007, 06, 223-231.	1.8	7
2500	Orbital currents in the Colle-Salvetti correlation energy functional and the degeneracy problem. <i>Journal of Chemical Physics</i> , 2007, 127, 124103.	1.2	11
2501	Evaluating the stability of disulfide bridges in proteins: a torsional potential energy surface for diethyl disulfide. <i>Molecular Simulation</i> , 2007, 33, 475-485.	0.9	39
2502	Quantum chemistry calculations for molecules coupled to reservoirs: Formalism, implementation, and application to benzenedithiol. <i>Journal of Chemical Physics</i> , 2007, 126, 174101.	1.2	94
2503	Modeling the adiabatic connection in H_2 . <i>Journal of Chemical Physics</i> , 2007, 126, 244104.	1.2	34
2504	Xe^{129} chemical shift by the perturbational relativistic method: Xenon fluorides. <i>Journal of Chemical Physics</i> , 2007, 127, 084312.	1.2	33

#	ARTICLE	IF	CITATIONS
2505	Significant increase in the stability of rare gas hydrides on insertion of beryllium atom. Journal of Chemical Physics, 2007, 127, 114314.	1.2	34
2506	Relativistic effects in the intermolecular interaction-induced nuclear magnetic resonance parameters of xenon dimer. Journal of Chemical Physics, 2007, 127, 164313.	1.2	36
2507	A density matrix-based method for the linear-scaling calculation of dynamic second- and third-order properties at the Hartree-Fock and Kohn-Sham density functional theory levels. Journal of Chemical Physics, 2007, 127, 204103.	1.2	55
2508	Theoretical understanding of the increment of \hat{I}^2 upon protonation of pyridine peripheral octupolar molecules: Toward nonlinear optical sensors. Journal of Chemical Physics, 2007, 127, 164704.	1.2	11
2509	Biatomic substrates for bulk-molecule interfaces: The PtCo-oxygen interface. Journal of Chemical Physics, 2007, 127, 244706.	1.2	15
2510	A general procedure to evaluate many-body spin operator amplitudes from periodic calculations: application to cuprates. New Journal of Physics, 2007, 9, 369-369.	1.2	17
2511	Density scaling and relaxation of the Pauli principle. Journal of Chemical Physics, 2007, 126, 124111.	1.2	4
2512	Assessment and formal properties of exchange-correlation functionals constructed from the adiabatic connection. Journal of Chemical Physics, 2007, 127, 034101.	1.2	59
2513	Range separated hybrid density functional with long-range Hartree-Fock exchange applied to solids. Journal of Chemical Physics, 2007, 127, 054101.	1.2	89
2514	A Review of Density Functional Theory Quantum Mechanics as Applied to Pharmaceutically Relevant Systems. Current Computer-Aided Drug Design, 2007, 3, 290-296.	0.8	28
2515	Theoretical Study of Decomposition Mechanism of Azoisobutyronitrile. Chinese Journal of Chemical Physics, 2007, 20, 224-232.	0.6	0
2516	Dissociative electron attachment and electron energy-loss spectra of phenyl azide. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 101-109.	0.6	14
2517	Non-Local Density Functional Description of Poly- Para -Phenylene Vinylene. Chinese Physics Letters, 2007, 24, 807-810.	1.3	6
2518	Density functional calculations of NMR shielding tensors for paramagnetic systems with arbitrary spin multiplicity: Validation on 3d metallocenes. Journal of Chemical Physics, 2007, 126, 024107.	1.2	98
2519	Self-interaction-corrected time-dependent density-functional-theory calculations of x-ray-absorption spectra. Physical Review A, 2007, 76, .	1.0	52
2520	Field-induced conformational changes in bimetallic oligoaniline junctions. Physical Review A, 2007, 75,	1.0	43
2521	Static and dynamic hyperpolarizability tensors of aluminum metal clusters, Al_4M_4	1.1	13
2522	3D-QSAR of Benzothiazole Derivatives as Potent Anticancer Agents. Chinese Journal of Chemical Physics, 2007, 20, 135-139.	0.6	7

#	ARTICLE	IF	CITATIONS
2523	Alternative perspective on density-functional perturbation theory. <i>Physical Review A</i> , 2007, 76, .	1.0	5
2524	Density functional theory investigation of 3d transition metal NMR shielding tensors in diamagnetic systems using the gauge-including projector augmented-wave method. <i>Physical Review B</i> , 2007, 76, .	1.1	27
2525	Effects of NH ₃ plasma pretreatment on initial reactions of atomic layer deposition TaN barrier layer on SiOC dielectric. <i>Applied Physics Letters</i> , 2007, 91, 242903.	1.5	1
2526	Conductance model of gold-molecule-silicon and carbon nanotube-molecule-silicon junctions. <i>Physical Review B</i> , 2007, 76, .	1.1	15
2527	The mechanism of DNA alkylation by the α -electrophilic center of nitrosamines and nitrosoureas: a theoretical study. , 2007, , .		0
2528	Transfer of signatures from the vibrational spectrum of benzene to a silicon complex. <i>Physical Review A</i> , 2007, 75, .	1.0	1
2529	Chiral plaquette polaron theory of cuprate superconductivity. <i>Physical Review B</i> , 2007, 76, .	1.1	10
2530	The importance of middle-range Hartree-Fock-type exchange for hybrid density functionals. <i>Journal of Chemical Physics</i> , 2007, 127, 221103.	1.2	152
2531	Atomic layer deposition of hafnium silicate gate dielectric layers. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2007, 25, 1302-1308.	0.9	23
2532	Structure, energy, and IR spectra of $(\text{H}_2\text{O})_n$ clusters ($n=1\text{--}8$): A theoretical study. <i>Journal of Chemical Physics</i> , 2007, 126, 034301.	1.2	21
2533	STUDY OF NANO-STRUCTURED SILICON-PHENYL NANOCLUSTERS TOWARDS SINGLE MOLECULE SENSING. <i>International Journal of High Speed Electronics and Systems</i> , 2007, 17, 327-338.	0.3	3
2534	Photoselected electron transfer pathways in DNA photolyase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 802-807.	3.3	70
2535	The Development of Computational Chemistry in Canada. <i>Reviews in Computational Chemistry</i> , 2007, , 213-299.	1.5	4
2536	On the performance of local, semilocal, and nonlocal exchange-correlation functionals on transition metal molecules. <i>Journal of Chemical Physics</i> , 2007, 126, 224105.	1.2	7
2537	Time-dependent density functional theory for nonlinear properties of open-shell systems. <i>Journal of Chemical Physics</i> , 2007, 127, 114101.	1.2	11
2538	Local hybrid functionals based on density matrix products. <i>Journal of Chemical Physics</i> , 2007, 127, 164117.	1.2	54
2539	A Local Structure Analysis of Molten Li ₂ CO ₃ Using the Density Functional Theory. <i>Electrochemistry</i> , 2007, 75, 466-471.	0.6	1
2540	Density Functional Methods in Biomolecular Modeling. <i>Reviews in Computational Chemistry</i> , 2007, , 217-259.	1.5	17

#	ARTICLE	IF	CITATIONS
2541	Chapter 1 Electrical characteristics of bulk-molecule interfaces. Theoretical and Computational Chemistry, 2007, 18, 1-33.	0.2	0
2542	Quantum Chemical Study on Stability and Reactivity of 1-Aminocyclopropane-1-carboxylic Acid Amine Radical Cation. Bulletin of the Chemical Society of Japan, 2007, 80, 1731-1739.	2.0	3
2543	The Synthesis, Structure and Properties of N-Acetylated Derivatives of Ethyl 3-Amino-1H-pyrazole-4-carboxylate. Chemical and Pharmaceutical Bulletin, 2007, 55, 747-752.	0.6	15
2544	DFT/Ab initio Study on the Pathways for the Reaction of CH ₃ SH with NO ₃ Radical. Chemistry Letters, 2007, 36, 400-401.	0.7	1
2545	Electronic Structure Calculations for Molecules Containing Transition Metals. Advances in Chemical Physics, 2007, , 333-387.	0.3	65
2546	The correlation between aromaticity and stability in planar N ₂ X ₂ (X = O, S, Se, and Te) Species. Molecular Physics, 2007, 105, 1883-1889.	0.8	5
2547	Multiscale modelling of carbon nanostructures. , 2007, , 220-260.		0
2548	Hole-vibronic coupling in oligothiophenes: impact of backbone torsional flexibility on relaxation energies. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2007, 365, 1435-1452.	1.6	59
2549	Role of Charge Transfer Interaction and Conjugation Length on Electrical Polarizability of Doped <i>trans</i> -Polyacetylene Oligomers. Journal of Physical Chemistry A, 2007, 111, 11867-11872.	1.1	2
2550	Tetrathiafulvalene-Based Materials for Organic Field Effect Transistors. Inspection of Their Semiconductor Properties by Means of Molecular Spectroscopy and Quantum Chemistry. Journal of Physical Chemistry C, 2007, 111, 10110-10118.	1.5	20
2551	Carbonyl mediated conductance through metal bound peptides: a computational study. Nanotechnology, 2007, 18, 424003.	1.3	12
2552	Dimerization of thymol blue in solution: Theoretical evidence. Talanta, 2007, 71, 1061-1067.	2.9	2
2553	Fingerprinting petroporphyrin structures with vibrational spectroscopy. Part 7. Calculations using density functional theory of the molecular structures and structure-sensitive vibrational modes of type II nickel(II) cycloalkanoporphyrins. Organic Geochemistry, 2007, 38, 250-266.	0.9	9
2554	Theoretical Study on Copper(I)-Catalyzed Cross-Coupling between Aryl Halides and Amides. Organometallics, 2007, 26, 4546-4554.	1.1	211
2555	Mechanism of [Pt(H ₂ SiV ₂ W ₁₀ O ₄₀) ₄]-Catalyzed Epoxidation of Alkenes with Hydrogen Peroxide. Inorganic Chemistry, 2007, 46, 1727-1736.	1.9	76
2556	Configurational stable propeller-like triarylphosphine and triarylphosphine oxide. Chemical Communications, 2007, , 3711.	2.2	39
2557	Resonance-Assisted Hydrogen Bonds: A Critical Examination. Structure and Stability of the Enols of β -Diketones and β -Enaminones. Journal of Physical Chemistry A, 2007, 111, 3585-3591.	1.1	142
2558	Quantum chemical calculations of equilibrium copper (I) isotope fractionations in ore-forming fluids. Chemical Geology, 2007, 243, 225-237.	1.4	86

#	ARTICLE	IF	CITATIONS
2559	Structural and electronic properties of lead chalcogenides from first principles. <i>Physical Review B</i> , 2007, 75, .	1.1	182
2560	Study on the binding of Thioflavin T to β -sheet-rich and non- β -sheet cavities. <i>Journal of Structural Biology</i> , 2007, 158, 358-369.	1.3	219
2561	Study of michael-michael-retro michael addition catalyzed by 9-amino-9-deoxyepiquinine using ESI-MS. <i>Journal of the American Society for Mass Spectrometry</i> , 2007, 18, 2074-2080.	1.2	19
2562	Solvation Effects on the Stability of Silver(I) Complexes with Pyridine-Containing Ligands Studied by Thermodynamic and DFT Methods. <i>Inorganic Chemistry</i> , 2007, 46, 4683-4691.	1.9	50
2563	General Performance of Density Functionals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10439-10452.	1.1	907
2564	Carbon-Hydrogen Bond Activation in Hydridotris(pyrazolyl)borate Platinum(IV) Complexes: Comparison of Density Functionals, Basis Sets, and Bonding Patterns. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2268-2281.	2.3	14
2565	Rational Design Based on Bioactive Conformation Analysis of Pyrimidinylbenzoates as Acetohydroxyacid Synthase Inhibitors by Integrating Molecular Docking, CoMFA, CoMSIA, and DFT Calculations. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 2335-2344.	2.5	50
2566	Composition dependence of structural and electronic properties of GaMnAs clusters from first principles. <i>Physical Review B</i> , 2007, 76, .	1.1	21
2567	Linear and Nonlinear Optical Properties of Pyridine-Based Octopolar Chromophores Designed for Chemical Sensing. Joint Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 18778-18784.	1.5	25
2568	Is Nucleus-Independent Chemical Shift Scan a Reliable Aromaticity Index for Planar Heteroatomic Ring Systems?. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9988-9994.	1.1	35
2569	Double-hybrid density functional theory for excited electronic states of molecules. <i>Journal of Chemical Physics</i> , 2007, 127, 154116.	1.2	404
2570	Density functional study of the conformations and intramolecular proton transfer in thiohydroxamic acids. <i>Organic and Biomolecular Chemistry</i> , 2007, 5, 547-557.	1.5	13
2571	Thiophene- and Selenophene-Based Heteroacenes: Combined Quantum Chemical DFT and Spectroscopic Raman and UV-Vis-NIR Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 7488-7496.	1.2	32
2572	Conformations of Proline Analogues Having Double Bonds in the Ring. <i>Journal of Physical Chemistry B</i> , 2007, 111, 5475-5482.	1.2	23
2573	Use of Constrained Synthetic Amino Acids in β -Helix Proteins for Conformational Control. <i>Journal of Physical Chemistry B</i> , 2007, 111, 3236-3242.	1.2	26
2574	A theoretical study of hydration effects on the prototropic tautomerism of selenouracils. <i>Organic and Biomolecular Chemistry</i> , 2007, 5, 3092.	1.5	22
2575	Rate Constants of Hydroperoxyl Radical Addition to Cyclic Nitrones: A DFT Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9995-10001.	1.1	30
2576	Intermediates in Dioxygen Activation by Methane Monooxygenase: A QM/MM Study. <i>Journal of the American Chemical Society</i> , 2007, 129, 3135-3147.	6.6	106

#	ARTICLE	IF	CITATIONS
2577	Stereoselective Quaternization of α -Amino Phenylacetonitriles Mediated by a Remote Sulfinyl Group. <i>Journal of Organic Chemistry</i> , 2007, 72, 5994-6005.	1.7	16
2578	Theoretical studies of Cu(i) sites in faujasite and their interaction with carbon monoxide. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5446.	1.3	37
2579	A Computational Study on the Stacking Interaction in Quinhydrone. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1998-2001.	1.1	42
2580	4-Aryl-1,3,2-oxathiazolium-5-olates as pH-Controlled NO-Donors: The Next Generation of S-Nitrosothiols. <i>Journal of the American Chemical Society</i> , 2007, 129, 5503-5514.	6.6	14
2581	H ₂ O ₃ as a Reactive Oxygen Species: Formation of 8-Oxoguanine from Its Reaction with Guanine. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4603-4615.	1.2	25
2582	Kinetic Analysis of the Pyrolysis of Phenethyl Phenyl Ether: Computational Prediction of β / α -Selectivities. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12118-12126.	1.1	64
2584	A well-tempered density functional theory of electrons in molecules. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2932.	1.3	344
2585	The Effects of Dissolved Halide Anions on Hydrogen Bonding in Liquid Water. <i>Journal of the American Chemical Society</i> , 2007, 129, 13847-13856.	6.6	416
2586	Chapter 8 Vibrational spectroscopy of gas-phase clusters and complexes. <i>Chemical Physics of Solid Surfaces</i> , 2007, , 327-375.	0.3	37
2587	Density-functional study of magnetism in bare Au nanoclusters: Evidence of permanent size-dependent spin polarization without geometry relaxation. <i>Physical Review B</i> , 2007, 75, .	1.1	30
2588	Optimized effective potentials from electron densities in finite basis sets. <i>Journal of Chemical Physics</i> , 2007, 127, 174101.	1.2	48
2589	Singlet-triplet gaps in large multireference systems: Spin-flip-driven alternatives for bioinorganic modeling. <i>Journal of Chemical Physics</i> , 2007, 126, 035102.	1.2	23
2590	Ground-state properties of multivalent manganese oxides: Density functional and hybrid density functional calculations. <i>Physical Review B</i> , 2007, 75, .	1.1	288
2591	The hydrolysis process of the anticancer complex [ImH][trans-RuCl ₄ (Im) ₂]: a theoretical study. <i>Dalton Transactions</i> , 2007, , 3507.	1.6	21
2592	Density Functional and Semiempirical Molecular Orbital Methods Including Dispersion Corrections for the Accurate Description of Noncovalent Interactions Involving Sulfur-Containing Molecules. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1656-1664.	2.3	73
2593	Dependence of Spurious Charge-Transfer Excited States on Orbital Exchange in TDDFT: Large Molecules and Clusters. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 976-987.	2.3	295
2594	Comparing the electron and hole mobilities in the β and β^2 phases of perylene: role of π -stacking. <i>Journal of Materials Chemistry</i> , 2007, 17, 1933-1938.	6.7	67
2595	Enhanced Fluorescence of Epicocconone in Surfactant Assemblies as a Consequence of Depth-Dependent Microviscosity. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1648-1656.	1.2	38

#	ARTICLE	IF	CITATIONS
2596	Synthesis of Bis(diarylphosphino)dithienosilole Derivatives as Novel Photo- and Electroluminescence Materials. <i>Organometallics</i> , 2007, 26, 6591-6595.	1.1	44
2597	Synthesis and Structures of Dinuclear 3,5-Bis(trifluoromethyl)pyrazolate Complexes of Ruthenium. <i>Organometallics</i> , 2007, 26, 6778-6783.	1.1	11
2598	Aromaticity and Curvature in Heteroacepentalenes. <i>Journal of Organic Chemistry</i> , 2007, 72, 4323-4327.	1.7	22
2599	Computational Studies of Radicals Relevant to Nucleic Acid Damage. <i>Advances in Quantum Chemistry</i> , 2007, 52, 89-120.	0.4	20
2600	Analytic derivatives for perturbatively corrected $\hat{\rho}$ -double hybrid density functionals: Theory, implementation, and applications. <i>Journal of Chemical Physics</i> , 2007, 126, 124115.	1.2	173
2601	Mechanistic Studies on the Stereoselective Formation of $\hat{1}^2$ -Mannosides from Mannosyl Iodides Using $\hat{1}\pm$ -Deuterium Kinetic Isotope Effects. <i>Journal of Organic Chemistry</i> , 2007, 72, 4663-4672.	1.7	58
2602	Electronic Nature of Planar Cyclobutenyl Dication Derivatives. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11904-11907.	1.1	10
2603	The role of ammonia in atomic layer deposition of tungsten nitride. <i>Applied Physics Letters</i> , 2007, 90, 173120.	1.5	17
2604	On the condensation mechanism of the dioxides of sixth-group elements: an ab initio approach. <i>Philosophical Magazine Letters</i> , 2007, 87, 979-988.	0.5	4
2605	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters: Benchmarks approaching the complete basis set limit. <i>Journal of Chemical Physics</i> , 2007, 127, 184104.	1.2	208
2606	Electroweak interactions in chiral molecules: two-component density functional theory study of vibrational frequency shifts in polyhalomethanes. <i>Molecular Physics</i> , 2007, 105, 41-49.	0.8	30
2607	Synthesis and characterization of a TTF- $\hat{1}$ -verdazyl radical—a new building block for conducting and/or magnetic systems. <i>New Journal of Chemistry</i> , 2007, 31, 1973.	1.4	26
2608	Improved accuracy with medium cost computational methods for the evaluation of bond length alternation of increasingly long oligoacetylenes. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5874.	1.3	55
2609	Theoretical investigation of the energies and geometries of photoexcited uranyl(VI) ion: A comparison between wave-function theory and density functional theory. <i>Journal of Chemical Physics</i> , 2007, 127, 214302.	1.2	75
2610	Energetics and Dynamics in MbCN: $\hat{1}$ CN-Vibrational Relaxation from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2007, 111, 218-226.	1.2	17
2611	Modulating Electronic Coupling Using O- and S-donor Linkers. <i>Inorganic Chemistry</i> , 2007, 46, 7840-7847.	1.9	28
2612	Theoretical Prediction of Intrinsic Self-Trapping of Electrons and Holes in Monoclinic $\langle \text{math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \langle \text{mml:msub} \langle \text{mml:mi} \text{HfO} \langle \text{mml:mi} \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \langle \text{mml:math} \rangle .$	2.9	133
2613	Which One among Zn(II), Co(II), Mn(II), and Fe(II) is the Most Efficient Ion for the Methionine Aminopeptidase Catalyzed Reaction?. <i>Journal of the American Chemical Society</i> , 2007, 129, 7776-7784.	6.6	57

#	ARTICLE	IF	CITATIONS
2614	Predicting the reactivity of ambidentate nucleophiles and electrophiles using a single, general-purpose, reactivity indicator. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2371.	1.3	40
2615	A tautomeric equilibrium between functionalized 2-formylphenylboronic acids and corresponding 1,3-dihydro-1,3-dihydroxybenzo[c][2,1]oxaboroles. <i>New Journal of Chemistry</i> , 2007, 31, 144-154.	1.4	51
2616	Effect of Ni(ii), Cu(ii) and Zn(ii) association on the keto-enol tautomerism of thymine in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2531-2537.	1.3	30
2617	Molecular recognition in molecular tweezers systems: quantum-chemical calculation of NMR chemical shifts. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4552.	1.3	21
2618	Reactivity of Ti(iv) species hosted in TS-1 towards H ₂ O ₂ in H ₂ O solutions investigated by ab initio cluster and periodic approaches combined with experimental XANES and EXAFS data: a review and new highlights. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4854.	1.3	198
2619	Chirality transfer through hydrogen-bonding: Experimental and ab initio analyses of vibrational circular dichroism spectra of methyl lactate in water. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 3127.	1.3	133
2620	Improved meta-GGA Correlation Functional of the Lap Family. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 746-754.	2.3	9
2621	Time-Dependent Density Functional Theory Study of the X-ray Absorption Spectroscopy of Acetylene, Ethylene, and Benzene on Si(100). <i>Journal of Physical Chemistry C</i> , 2007, 111, 3333-3340.	1.5	76
2622	Comparison of Static First Hyperpolarizabilities Calculated with Various Quantum Mechanical Methods. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1319-1327.	1.1	125
2623	DFT Method Estimation of Standard Redox Potential of Metal Ions and Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 789-795.	2.3	36
2624	Comparative Reactivity of TpRu(L)(NCMe)Ph (L = CO or PMe ₃): Impact of Ancillary Ligand L on Activation of Carbon-Hydrogen Bonds Including Catalytic Hydroarylation and Hydrovinylation/Oligomerization of Ethylene. <i>Journal of the American Chemical Society</i> , 2007, 129, 6765-6781.	6.6	99
2625	Comparative Performance of Exchange and Correlation Density Functionals in Determining Intermolecular Interaction Potentials of the Methane Dimer. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9586-9590.	1.1	17
2626	Redox and Functional Analysis of the Rieske Ferredoxin Component of the Toluene 4-Monooxygenase. <i>Biochemistry</i> , 2007, 46, 976-986.	1.2	20
2627	Push-Pull Bithienyl Chromophore with an Unusual Transverse Path of Conjugation. <i>Journal of Physical Chemistry A</i> , 2007, 111, 841-851.	1.1	5
2628	On the Bonding of First-Row Transition Metal Cations to Guanine and Adenine Nucleobases. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9823-9829.	1.1	34
2629	Phosphine Adsorption on the In-Rich InP(001) Surface: Evidence of Surface Dative Bonds at Room Temperature. <i>Langmuir</i> , 2007, 23, 10109-10115.	1.6	7
2630	Electronic and Molecular Structures of Trigonal Truxene-Core Systems Conjugated to Peripheral Fluorene Branches. Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4026-4035.	1.2	36
2631	STRUCTURE, VIBRATIONAL PROPERTIES AND POLARIZABILITIES OF METHYLNAPHTHALENE ISOMERS. A QUANTUM-MECHANICAL APPROACH. <i>Polycyclic Aromatic Compounds</i> , 2007, 27, 65-94.	1.4	19

#	ARTICLE	IF	CITATIONS
2632	Equilibrium Geometries and Structural Stability of the Al _m Na _n (<i>m</i> = 2 ⁴ ; <i>n</i> = 1 ⁸) Clusters. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1818-1829.	2.3	12
2633	An Experimental and Computational Analysis on the Differential Role of the Positional Isomers of Symmetric Bis-2-(pyridyl)-1H-benzimidazoles as DNA Binding Agents. <i>Journal of Organic Chemistry</i> , 2007, 72, 1912-1923.	1.7	82
2634	Computational Studies of EPR Parameters for Paramagnetic Molybdenum Complexes. II. Larger MoV Systems Relevant to Molybdenum Enzymes. <i>Inorganic Chemistry</i> , 2007, 46, 8146-8161.	1.9	27
2635	Electron and hole mobilities in polymorphs of benzene and naphthalene: Role of intermolecular interactions. <i>Journal of Chemical Physics</i> , 2007, 126, 144710.	1.2	78
2636	Electron Transport through Heterogeneous Intermolecular Tunnel Junctions. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1535-1540.	1.5	7
2637	Structural Evidence of the Similarity of Sb(OH) ₃ and As(OH) ₃ with Glycerol: Implications for Their Uptake. <i>Chemical Research in Toxicology</i> , 2007, 20, 1269-1276.	1.7	84
2638	Insights into Mechanistic Photodissociation of Acetyl Chloride by ab Initio Calculations and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9355-9361.	1.1	11
2639	Density Functional Theory Study of Anode Reactions on Pt-Based Alloy Electrodes. <i>Journal of Physical Chemistry C</i> , 2007, 111, 272-279.	1.5	28
2640	Atomic Partitioning of the Dissociation Energy of the P=O(H) Bond in Hydrogen Phosphate Anion (HPO ₄ ²⁻): Disentangling the Effect of Mg ²⁺ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 8864-8872.	1.1	43
2641	Simple Methods To Reduce Charge-Transfer Contamination in Time-Dependent Density-Functional Calculations of Clusters and Liquids. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1680-1690.	2.3	93
2642	DNA Oligonucleotide cis-Platin Binding: Ab Initio Interpretation of the Vibrational Spectra. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9714-9723.	1.1	33
2643	Restricted Ensemble-Referenced Kohn-Sham versus Broken Symmetry Approaches in Density Functional Theory: Magnetic Coupling in Cu Binuclear Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 764-774.	2.3	113
2644	A Rare Dimer of Dimers Having Four Hydride Linkers Joining Two Quadruply Bonded Dimolybdenum Units. <i>Inorganic Chemistry</i> , 2007, 46, 6858-6863.	1.9	9
2645	Structural, Infrared, and Density Functional Theory Studies of N,N,N',N'-Tetramethylimidazolidinium Dichloride: A Model for Cation-Anion Association of Headgroups and Counterions in the Interfacial Regions of Gemini Micelles. <i>Journal of Physical Chemistry B</i> , 2007, 111, 13668-13674.	1.2	2
2646	Characterization of Dihydro-A2PE: An Intermediate in the A2E Biosynthetic Pathway. <i>Biochemistry</i> , 2007, 46, 10122-10129.	1.2	28
2647	Density Functional Study of the Dissociative Adsorption of Aromatic Molecules on the Si(100) Surface: On the Way from Benzene to Larger Polycyclic Hydrocarbons. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1392-1401.	1.5	8
2648	Representative Benchmark Suites for Barrier Heights of Diverse Reaction Types and Assessment of Electronic Structure Methods for Thermochemical Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 569-582.	2.3	207
2649	The Catalytic Effect of Dihydrofolate Reductase and Its Mutants Is Determined by Reorganization Energies. <i>Biochemistry</i> , 2007, 46, 6011-6025.	1.2	92

#	ARTICLE	IF	CITATIONS
2650	The Presumption of Innocence? A DFT-Directed Verdict on Oxidized Amavadin and Vanadium Catecholate Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 11297-11307.	1.9	21
2651	Hydrogen detachment of the hexahydrated hydroiodic acid upon attaching an excess electron. <i>Molecular Physics</i> , 2007, 105, 2577-2581.	0.8	3
2652	Evidence for Strong Tantalum-to-Boron Dative Interactions in (silox) ₃ Ta(BH ₃) and (silox) ₃ Ta(̄-2-B,Cl-BCl ₂ Ph) (silox =tBu ₃ SiO)1. <i>Inorganic Chemistry</i> , 2007, 46, 1222-1232.	1.9	42
2653	Theoretical Design of an Aromatic Hydrocarbon Rotor Driven by a Circularly Polarized Electric Field. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9374-9378.	1.1	8
2654	Computational Study of the Zr ⁴⁺ Tetranuclear Polymer, [Zr ₄ (OH) ₈ (H ₂ O) ₁₆] ⁸⁺ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 11395-11399.	1.1	22
2655	Ab Initio Analysis of Electron Transport in Oligoglycines. <i>Journal of Physical Chemistry C</i> , 2007, 111, 14552-14559.	1.5	16
2656	Theoretical Study of Cycloaddition Reactions of Heavy Carbenes with C ₆₀ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 6232-6240.	1.1	19
2657	Theoretical and Experimental Studies of the Spin Trapping of Inorganic Radicals by 5,5-Dimethyl-1-Pyrroline N-Oxide (DMPO). 2. Carbonate Radical Anion. <i>Journal of Physical Chemistry A</i> , 2007, 111, 384-391.	1.1	78
2658	Nitrogen Fixation by a Molybdenum Catalyst Mimicking the Function of the Nitrogenase Enzyme: A Critical Evaluation of DFT and Solvent Effects. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1708-1720.	2.3	52
2659	Hydrogen Bonding Mediated by Key Orbital Interactions Determines Hydration Enthalpy Differences of Phosphate Water Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10804-10814.	1.1	10
2660	Theoretical Study of the Phosphotriesterase Reaction Mechanism. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1253-1255.	1.2	105
2661	Quartic-Scaling Analytical Energy Gradient of Scaled Opposite-Spin Second-Order Møller-Plesset Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 988-1003.	2.3	44
2662	O-H Bond Dissociation Enthalpies of Oximes: A Theoretical Assessment and Experimental Implications. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13112-13125.	1.1	34
2663	First-principle studies of the geometries and electronic properties of Cu _m Si _n (2 ≤ m + n ≤ 7) clusters. <i>Chinese Physics B</i> , 2007, 16, 3359-3369.		13
2664	Performance of modern density functional theory for the prediction of hyperfine structure: meta-GGA and double hybrid functionals. <i>Molecular Physics</i> , 2007, 105, 2049-2071.	0.8	129
2665	Beyond Exciton Theory: A Time-Dependent DFT and Franck-Condon Study of Perylene Diimide and Its Chromophoric Dimer. <i>Journal of the American Chemical Society</i> , 2007, 129, 7586-7595.	6.6	148
2666	Characterization of the Tyrosine-Z Radical and Its Environment in the Spin-Coupled S ₂ TyrZ State of Photosystem II from <i>Thermosynechococcus elongatus</i> . <i>Biochemistry</i> , 2007, 46, 3138-3150.	1.2	35
2667	Assessment of time-dependent density functional schemes for computing the oscillator strengths of benzene, phenol, aniline, and fluorobenzene. <i>Journal of Chemical Physics</i> , 2007, 127, 084103.	1.2	85

#	ARTICLE	IF	CITATIONS
2668	Spectroscopic and Computational Studies of Ni ³⁺ Complexes with Mixed S/N Ligation: Implications for the Active Site of Nickel Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2007, 46, 8511-8523.	1.9	22
2669	Reduction of Titanium Supported by a σ -Bonded Tripyrrole Ligand: Ligand C-N Bond Cleavage and Coordination of Olefin and Arene with an Inverse Sandwich Structure. <i>Organometallics</i> , 2007, 26, 48-55.	1.1	40
2670	A Computational Study on the Interaction of the Nitric Oxide Ions NO ⁺ and NO ⁻ with the Side Groups of the Aromatic Amino Acids. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1981-1989.	1.1	13
2671	Theoretical Design of Low Band Gap Conjugated Polymers through Ladders with Acetylenic Crosspieces. <i>Macromolecules</i> , 2007, 40, 6740-6747.	2.2	15
2672	Intrinsic Flexing Abilities of Molecular Muscles Based on Tetrakis(2,3-thienylene): A Quantum Mechanical Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2329-2335.	1.1	4
2673	Detection and Determination of the {Fe(NO) ₂ } Core Vibrational Features in Dinitrosyl Iron Complexes from Experiment, Normal Coordinate Analysis, and Density Functional Theory: An Avenue for Probing the Nitric Oxide Oxidation State. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2335-2346.	1.2	25
2674	Structural Transitions from Pyramidal to Fused Planar to Tubular to Core/Shell Compact in Gold Clusters: Au _n ⁻ (n = 21-25). <i>Journal of Physical Chemistry C</i> , 2007, 111, 4190-4198.	1.5	85
2675	Ca ²⁺ Selectivity of the Sarcoplasmic Reticulum Ca ²⁺ ATPase at the Enzyme-Water Interface and in the Ca ²⁺ Entrance Channel. <i>Journal of Physical Chemistry B</i> , 2007, 111, 12282-12293.	1.2	5
2676	Ab Initio Thermochemistry of the Hydrogenation of Hydrocarbon Radicals Using Silicon-, Germanium-, Tin-, and Lead-Substituted Methane and Isobutane. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8677-8688.	1.1	12
2677	Comparative Theoretical Study of Heterocyclic Conducting Oligomers: Neutral and Oxidized Forms. <i>Journal of Physical Chemistry C</i> , 2007, 111, 4823-4830.	1.5	67
2678	Electronic Structure and Bonding of {Fe(PhNO ₂) ₆ } Complexes: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3571-3576.	1.1	4
2679	Interpretation of Synchrotron Radiation Circular Dichroism Spectra of Anionic, Cationic, and Zwitterionic Alanine Forms. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2750-2760.	1.1	33
2680	Electronic and Vibrational Spectroscopies Applied to Organic/Inorganic Interfaces. <i>Chemical Reviews</i> , 2007, 107, 1161-1232.	23.0	149
2681	Theoretical Investigation on the Electronic and Geometric Structure of GaN ₂ ⁺ and GaN ₄ ⁺ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 8892-8902.	1.1	8
2682	Is the Peptide Bond Formation Activated by Cu ²⁺ Interactions? Insights from Density Functional Calculations. <i>Journal of Physical Chemistry B</i> , 2007, 111, 5740-5747.	1.2	32
2683	Helically Annelated and Cross-Conjugated β -Oligothiophenes: A Fourier Transform Raman Spectroscopic and Quantum Chemical Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 4854-4860.	1.5	14
2684	Thermochemical Kinetics of Hydrogen-Atom Transfers between Methyl, Methane, Ethynyl, Ethyne, and Hydrogen. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4632-4642.	1.1	59
2685	Creating Quaternary Centers with High Exo Stereoselectivity Using Activated β -Alkynyl Dienophiles. <i>Journal of the American Chemical Society</i> , 2007, 129, 10078-10079.	6.6	18

#	ARTICLE	IF	CITATIONS
2686	Acidity and Proton Affinity of Hypoxanthine in the Gas Phase versus in Solution: An Intrinsic Reactivity and Biological Implications. <i>Journal of Organic Chemistry</i> , 2007, 72, 6548-6555.	1.7	48
2687	Extension of the Core-Valence-Rydberg B3LYP Functional to Core-Excited-State Calculations of Third-Row Atoms. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1295-1305.	2.3	46
2688	Development, Mechanism, and Scope of the Palladium-Catalyzed Enantioselective Allene Diboration. <i>Journal of the American Chemical Society</i> , 2007, 129, 8766-8773.	6.6	160
2689	Can the DFT-D method describe the full range of noncovalent interactions found in large biomolecules?. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 448-451.	1.3	123
2690	Multidimensional Quantum Dynamical Study of \hat{I}^2 -Hydrogen Transfer in a Cationic Rhodium Complex. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2407-2419.	1.1	7
2691	Hyperfine Coupling in Methyl Radical Isotopomers. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10625-10634.	1.1	19
2692	Theoretical Study on Photophysical Properties of Phenolpyridyl Boron Complexes. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2739-2744.	1.1	38
2693	Effects of the 3- and 4-Methoxy and Acetamide Substituents and Solvent Environment on the Electronic Properties of N-Substituted 1,8-Naphthalimide Derivatives. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9724-9732.	1.1	24
2694	Ab Initio Study on the Kinetics of Hydrogen Abstraction for the $H + \text{Alkene} \rightarrow H_2 + \text{Alkenyl}$ Reaction Class. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2156-2165.	1.1	29
2695	Silicon-Carbon Unsaturated Compounds. 72. Thermolysis of Acylpolysilanes with Diphenylketene. <i>Organometallics</i> , 2007, 26, 5535-5542.	1.1	4
2696	Characterization of the Nitrosyl Adduct of Substrate-Bound Mouse Cysteine Dioxygenase by Electron Paramagnetic Resonance: A Detailed Electronic Structure of the Active Site and Mechanistic Implications. <i>Biochemistry</i> , 2007, 46, 8569-8578.	1.2	99
2697	Synthesis, Structure, and LLCT Transitions in Terminal Hydrazido($2\lambda^2$) Bipyridine Complexes of Titanium. <i>Inorganic Chemistry</i> , 2007, 46, 6373-6381.	1.9	45
2698	Direct Dynamics Studies on Hydrogen Abstraction Reactions of $CH_3CH_2CH_3$ and $CH_3CH_2CH_2CH_2F$ with OH Radicals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7761-7770.	1.1	13
2699	Enhancement in Electronic Communication upon Replacement of Mo=O by Mo=S Bonds in Tetranuclear Clusters of the Type $[Mo_2]_2(\mu_4-E)_2$ (E = O or S). <i>Inorganic Chemistry</i> , 2007, 46, 9294-9302.	1.9	13
2700	Intrinsic Conformational Characteristics of \pm -Diphenylglycine. <i>Journal of Organic Chemistry</i> , 2007, 72, 2174-2181.	1.7	24
2701	Experimental and Theoretical Charge Density Distribution in Two Ternary Cobalt(III) Complexes of Aromatic Amino Acids. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10123-10133.	1.1	19
2702	Comparison of Density Functionals for Reactions of Sulfur Ylides with Aldehydes and Olefins. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12019-12025.	1.1	9
2703	Reaction of Acetaldehyde with Ni: An Extended Theoretical Study of the Decarbonylation Mechanism of Acetaldehyde by First-Row Transition Metal Ions. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3566-3570.	1.1	24

#	ARTICLE	IF	CITATIONS
2704	Enantioselective Synthesis of Chiral Sulfones by Rh-Catalyzed Asymmetric Addition of Boronic Acids to $\hat{1}\pm, \hat{1}^2$ -Unsaturated 2-Pyridyl Sulfones. <i>Journal of Organic Chemistry</i> , 2007, 72, 9924-9935.	1.7	94
2705	The Conformations of 13-Vertex ML ₂ C ₂ B ₁₀ Metallocarboranes: An Experimental and Computational Studies. <i>Journal of the American Chemical Society</i> , 2007, 129, 3302-3314.	6.6	21
2706	Bonding Analyses, Formation Energies, and Vibrational Properties of M ⁿ⁺ R ₂ Complexes (M = Ag(I), Ni(II), Cu(II), or Zn(II)). <i>Journal of Physical Chemistry A</i> , 2007, 111, 13075-13087.	1.1	31
2707	A Fractional Bond Order of 1/2 in Pd ²⁺ Formamidinate Species; The Value of Very High-Field EPR Spectra. <i>Journal of the American Chemical Society</i> , 2007, 129, 1393-1401.	6.6	49
2708	Proper Choice of XC Functionals and Calculations of Fluorescence-Emitting Energies for Coumarin Derivatives. <i>Acta Physico-chimica Sinica</i> , 2007, 23, 1831-1838.	0.6	11
2709	DFT Investigations About Pyrazine Molecules on Si(100)-2 \times 1 Surface. <i>Chemical Research in Chinese Universities</i> , 2007, 23, 444-451.	1.3	2
2710	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. <i>Physical Review B</i> , 2007, 75, .	1.1	306
2711	Structural and Electronic Properties of Polyacetylene and Polyynes from Hybrid and Coulomb-Attenuated Density Functionals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11930-11935.	1.1	139
2712	Single-molecule field-effect transistors: A computational study of the effects of contact geometry and gating-field orientation on conductance-switching properties. <i>Physical Review B</i> , 2007, 75, .	1.1	18
2713	The Role of Charge Localization in Current-Driven Dynamics. <i>Israel Journal of Chemistry</i> , 2007, 47, 99-104.	1.0	5
2714	Local hybrid functionals: An assessment for thermochemical kinetics. <i>Journal of Chemical Physics</i> , 2007, 127, 194102.	1.2	87
2715	A Density Functional Study of Methanol Clusters. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 54-61.	2.3	128
2716	Density Functionals for Noncovalent Interaction Energies of Biological Importance. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 289-300.	2.3	557
2717	Exploring pathways and barriers for coupled ET/PT in cytochrome c oxidase: A general framework for examining energetics and mechanistic alternatives. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2007, 1767, 244-260.	0.5	45
2718	The influence of hydrogen bonds on electron transfer rate in photosynthetic RCs. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2007, 1767, 541-549.	0.5	28
2719	Polymorphs and a pseudo-polymorphs based on a luminescent boron-containing compound: structural diversity arising from conformational isomers and noncovalent interactions. <i>CrystEngComm</i> , 2007, 9, 951.	1.3	13
2720	Dehydrogenation of Light Alkanes over Isolated Gallyl Ions in Ga/ZSM-5 Zeolites. <i>Journal of Physical Chemistry C</i> , 2007, 111, 13068-13075.	1.5	87
2721	A Theoretical Study on the Hydrolysis Process of the Antimetastatic Ruthenium(III) Complex NAMI-A. <i>Journal of Physical Chemistry B</i> , 2007, 111, 7862-7869.	1.2	54

#	ARTICLE	IF	CITATIONS
2722	Minimum Energy Pathways for Proton Transfer between Adjacent Sites Exposed to Water. <i>Journal of Physical Chemistry B</i> , 2007, 111, 6059-6070.	1.2	23
2723	Modeling Mechanisms of Unusual Benzene Imine N6 Adduct Formation in Carcinogenic Reactions of Arylnitrenium Ions with Adenosine. <i>Journal of Organic Chemistry</i> , 2007, 72, 10058-10064.	1.7	5
2724	Why does the B3LYP hybrid functional fail for metals?. <i>Journal of Chemical Physics</i> , 2007, 127, 024103.	1.2	481
2725	A Kinetic and Thermodynamic Study of the Glycosidic Bond Cleavage in Deoxyuridine. <i>Journal of Physical Chemistry B</i> , 2007, 111, 3800-3812.	1.2	35
2726	Concurrent Cyclopropanation by Carbenes and Carbanions? A Density Functional Theory Study on the Reaction Pathways. <i>Journal of Organic Chemistry</i> , 2007, 72, 5139-5145.	1.7	11
2727	London dispersion forces by range-separated hybrid density functional with second order perturbational corrections: The case of rare gas complexes. <i>Journal of Chemical Physics</i> , 2007, 126, 044103.	1.2	73
2728	Theoretical Study of Reaction Mechanisms of OH Radical with Toluene 1,2-Epoxyde/2-Methyloxepin. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13088-13098.	1.1	11
2729	Unusual substituent effects on the bonding of iminoboranes. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 3970-3977.	1.3	31
2730	Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry. <i>Reviews in Computational Chemistry</i> , 2007, , 1-86.	1.5	775
2731	Theoretical Study of Metal-Ligand Interaction in Sm(III), Eu(III), and Tb(III) Complexes of Coumarin-3-Carboxylic Acid in the Gas Phase and Solution. <i>Inorganic Chemistry</i> , 2007, 46, 10926-10936.	1.9	27
2732	Electronically excited water aggregates and the adiabatic band gap of water. <i>Journal of Chemical Physics</i> , 2007, 126, 014509.	1.2	20
2733	How Many Drugs Are Catecholics. <i>Molecules</i> , 2007, 12, 878-884.	1.7	52
2734	Hydrogen-Atom Transfer in Open-Shell Organometallic Chemistry: The Reactivity of Rh(II)(cod) and Ir(II)(cod) Radicals. <i>Chemistry - A European Journal</i> , 2007, 13, 3386-3405.	1.7	50
2735	Silica Gel Triggered Transformations of 3-Methylenecyclopropylmethyl Sulfonates to 3-Methylenecyclobutyl Analogues: Experimental and Computational Studies. <i>Chemistry - A European Journal</i> , 2007, 13, 862-869.	1.7	25
2736	The Preferred Reaction Path for the Oxidation of Methanol by PQQ-Containing Methanol Dehydrogenase: Addition vs. Elimination versus Hydride-Transfer Mechanism. <i>Chemistry - A European Journal</i> , 2007, 13, 2109-2117.	1.7	48
2737	Contraction Process of an Electroactive Actuator Based on a One Microsecond Atomistic Molecular Dynamics Simulation. <i>Chemistry - A European Journal</i> , 2007, 13, 2695-2700.	1.7	7
2738	Di(benzothiazol-2-yl)phosphanide as a Janus-Head Ligand to Caesium. <i>Chemistry - A European Journal</i> , 2007, 13, 3636-3642.	1.7	37
2739	Formation of the Active Species of Cytochrome P450 by Using Iodosylbenzene: A Case for Spin-Selective Reactivity. <i>Chemistry - A European Journal</i> , 2007, 13, 4103-4115.	1.7	46

#	ARTICLE	IF	CITATIONS
2740	Cycloaddition Reactions of 16-Electron d ⁴ Metallocene Complexes with C ₆₀ : A Theoretical Study. Chemistry - A European Journal, 2007, 13, 6171-6178.	1.7	10
2741	π-π Stacking versus Steric Effects in Stereoselectivity Control: Highly Diastereoselective Synthesis of syn-1,2-Diarylpropylamines. Chemistry - A European Journal, 2007, 13, 6179-6195.	1.7	57
2742	Ring-Borylated 15-Electron and 17-Electron ansa-Chromocene Complexes, their Physical Properties and Molecular Structures. Chemistry - A European Journal, 2007, 13, 6212-6222.	1.7	7
2743	Selective Treatment of Cancer: Synthesis, Biological Evaluation and Structural Elucidation of Novel Analogues of the Antibiotic CC-1065 and the Duocarmycins. Chemistry - A European Journal, 2007, 13, 4396-4409.	1.7	38
2744	Kinetic and Thermochemical Study of the Antioxidant Activity of Sulfur-Containing Analogues of Vitamin E. Chemistry - A European Journal, 2007, 13, 8223-8230.	1.7	42
2745	How Can a Carbon Atom Be Covalently Bound to Five Ligands? The Case of Si ₂ (CH ₃) ₇ ⁺ . Angewandte Chemie - International Edition, 2007, 46, 381-385.	7.2	24
2746	Acid Initiation of Ammonia-Borane Dehydrogenation for Hydrogen Storage. Angewandte Chemie - International Edition, 2007, 46, 746-749.	7.2	375
2747	Enantioselective Organocatalytic Conjugate Addition of N ⁺ -Heterocycles to α,β -Unsaturated Aldehydes. Angewandte Chemie - International Edition, 2007, 46, 1983-1987.	7.2	180
2748	Asymmetric Crystal Growth of α -Resorcinol from the Vapor Phase: Surface Reconstruction and Conformational Change Are the Culprits. Angewandte Chemie - International Edition, 2007, 46, 5537-5540.	7.2	18
2749	Spirodiepoxides: Heterocycle Synthesis and Mechanistic Insight. Angewandte Chemie - International Edition, 2007, 46, 7108-7111.	7.2	29
2750	Sixty Years after Wittig: Gas-Phase Synthesis of Lithium Trimethylammonium Methylide, [(CH ₃) ₃ NCH ₂ Li] ⁺ . Angewandte Chemie - International Edition, 2007, 46, 7048-7051.	7.2	27
2755	Spirodiepoxides: Heterocycle Synthesis and Mechanistic Insight. Angewandte Chemie, 2007, 119, 7238-7241.	1.6	5
2756	Sixty Years after Wittig: Gas-Phase Synthesis of Lithium Trimethylammonium Methylide, [(CH ₃) ₃ NCH ₂ Li] ⁺ . Angewandte Chemie, 2007, 119, 7178-7181.	1.6	12
2758	Improved Synthesis of Pyrroles and Indoles via Lewis Acid-Catalyzed Mukaiyama-Michael-Type Addition/Heterocyclization of Enolsilyl Derivatives on 1,2-Diaza-1,3-Butadienes. Role of the Catalyst in the Reaction Mechanism. Advanced Synthesis and Catalysis, 2007, 349, 907-915.	2.1	33
2759	Theoretical Studies on ortho-Oxidation of Phenols with Dioxygen Mediated by Dicopper Complex: Hints for a Catalyst with the Phenolase Activity of Tyrosinase. Advanced Synthesis and Catalysis, 2007, 349, 595-600.	2.1	12
2760	Asymmetric Total Synthesis of Nigerone and Nigronone: Enantioselective Oxidative Biaryl Coupling of Highly Hindered Naphthols. Advanced Synthesis and Catalysis, 2007, 349, 583-594.	2.1	63
2761	Memory Effects in Palladium-Catalyzed Allylic Alkylations of α -Cyclohexenyl Acetate. Advanced Synthesis and Catalysis, 2007, 349, 2631-2640.	2.1	27
2762	Synthesis, Characterization, and DNA-Binding Properties of the Chiral Ruthenium(II) Complexes λ^1 - and λ^2 -[Ru(bpy) ₂ (dmppd)] ²⁺ (dmppd = 10,12-Dimethylpteridino[6,7-f][1,10]phenanthroline-11,13(10H,12H)-dione). Tj ETQ		

#	ARTICLE	IF	CITATIONS
2763	Experimental and Density Functional Theory (DFT) Studies on the DNA-Binding Trend and Spectral Properties of the Ruthenium Complexes $[\text{Ru}(\text{4,7-dmp})(\text{bdip})]^{2+}$ and $[\text{Ru}(\text{bpy})_2(\text{bdip})]^{2+}$ (4,7-dmp=4,7-dimethyl-1,10-phenanthroline,) <i>Tj ETQq0 0 0 rg BT /Overlock 10 Tf 5 Helvetica Chimica Acta</i> , 2007, 90, 1786-1801.		
2764	Comparison of basis set effects and the performance of ab initio and DFT methods for probing equilibrium fluctuations. <i>Journal of Computational Chemistry</i> , 2007, 28, 478-490.	1.5	19
2765	Density functional theory augmented with an empirical dispersion term. Interaction energies and geometries of 80 noncovalent complexes compared with ab initio quantum mechanics calculations. <i>Journal of Computational Chemistry</i> , 2007, 28, 555-569.	1.5	620
2766	Theoretical study and rate constant calculation for reaction of $\text{CF}_3\text{CH}_2\text{OH}$ with OH. <i>Journal of Computational Chemistry</i> , 2007, 28, 802-810.	1.5	14
2767	New insights on the bridge carbon-carbon bond in propellanes: A theoretical study based on the analysis of the electron localization function. <i>Journal of Computational Chemistry</i> , 2007, 28, 857-864.	1.5	47
2768	Description of core excitations by time-dependent density functional theory with local density approximation, generalized gradient approximation, meta-generalized gradient approximation, and hybrid functionals. <i>Journal of Computational Chemistry</i> , 2007, 28, 2067-2074.	1.5	43
2769	Geometry optimization using generalized, chemically meaningful constraints. <i>Journal of Computational Chemistry</i> , 2007, 28, 2226-2236.	1.5	90
2770	A self-contained and portable density functional theory library for use in ab initio quantum chemistry programs. <i>Journal of Computational Chemistry</i> , 2007, 28, 2569-2575.	1.5	22
2771	Competing Radical and Non-Radical Pathways for the Decomposition of $\text{LFell}(\text{H}_2\text{O}_2)$ Complexes: a Density Functional Study. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 65-73.	1.0	15
2772	Synthesis, Structure and Reactivity of Trimethylsilyl-Substituted Phosphametalloenes. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 553-561.	1.0	17
2773	Redox-Induced Phase Transition in $\text{Pt}(\text{bpy})\text{Cl}_2$: Spectroscopic Study Supported by DFT Calculations. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 5735-5742.	1.0	14
2774	Polyazaacenes - On the Way to Stable, Fluorescent and Redox-Active Derivatives. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 1237-1243.	1.2	28
2775	Synthesis and Structural Investigation of C_4 - and C_2 -Symmetric Molecular Scaffolds Based on Imidazole Peptides. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 1779-1792.	1.2	33
2776	Stereospecific Side Chain Activation in Cyclobutadiene- $\text{Fe}(\text{CO})_3$ Chemistry: A Theoretical and Experimental Study on the Structure and Configurational Stability of Cationic, Radical and Anionic Intermediates. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 3991-3998.	1.2	7
2777	Insights into the Molecular Structure and Reactivity of I^{\pm} -Dialkoxy-Substituted Ethyne and Butadiyne. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 5834-5839.	1.2	10
2778	What can we learn from two-center three-electron bonding with the topological analysis of ELF?. <i>Heteroatom Chemistry</i> , 2007, 18, 135-160.	0.4	52
2779	Fourier Transform Raman and DFT Study of Three Annulated Oligothiophenes with Different Molecular Shapes. <i>ChemPhysChem</i> , 2007, 8, 745-750.	1.0	6
2780	Gas-Phase Reactions Between Thiourea and Ca^{2+} : New Evidence for the Formation of $[\text{Ca}(\text{NH}_3)]^{2+}$ and Other Doubly Charged Species. <i>ChemPhysChem</i> , 2007, 8, 1330-1337.	1.0	25

#	ARTICLE	IF	CITATIONS
2781	Ab Initio Static and Molecular Dynamics Study of 4-Styrylpyridine. <i>ChemPhysChem</i> , 2007, 8, 1402-1416.	1.0	12
2782	Non-Resonance-Assisted Hydrogen Bonding in Hydroxymethylene and Aminomethylene Cyclobutanones and Cyclobutenones and Their Nitrogen Counterparts.. <i>ChemPhysChem</i> , 2007, 8, 1950-1958.	1.0	82
2783	Alk-1-ene Polymerization in the Presence of a Monocyclopentadienyl Zirconium(IV) Acetamidinate Catalyst: Microstructural and Mechanistic Insights. <i>Macromolecular Rapid Communications</i> , 2007, 28, 1128-1134.	2.0	22
2784	Thermochemistry, bonding, and reactivity of Ni + and Ni 2+ in the gas phase. <i>Mass Spectrometry Reviews</i> , 2007, 26, 474-516.	2.8	36
2785	Mass-selective vibrational spectroscopy of vanadium oxide cluster ions. <i>Mass Spectrometry Reviews</i> , 2007, 26, 542-562.	2.8	192
2786	¹ H, ¹³ C and ¹⁵ N NMR coordination shifts in gold(III), cobalt(III), rhodium(III) chloride complexes with pyridine, 2,2'-bipyridine and 1,10-phenanthroline. <i>Magnetic Resonance in Chemistry</i> , 2007, 45, 24-36.	1.1	59
2787	Direct ab initio dynamics calculations of the rate constants for the reaction of CHF ₂ CF ₂ OCH ₃ with Cl. <i>International Journal of Chemical Kinetics</i> , 2007, 39, 221-230.	1.0	1
2788	Spectroscopic and computational studies on self-assembly complexes of bis(pyrrol-2-yl)ethane. <i>Journal of Physical Chemistry B</i> , 2007, 11, 483-495.	1.2	6
2789	Adsorption and thermal chemistry of 1,1,1,5,5,5-hexafluoro-2,4-pentanedione (hfacH) and (hexafluoroacetylacetonate)Cu(vinyltrimethylsilane) ((hfac)Cu(VTMS)) on TiCN-covered Si(100) surface. <i>Surface Science</i> , 2007, 601, 155-164.	0.8	22
2790	The molecular orientation of DNA bases on H-passivated Si(111) surfaces investigated by means of near edge X-ray absorption fine structure spectroscopy. <i>Surface Science</i> , 2007, 601, 2291-2296.	0.8	16
2791	Interaction of 2,2,6,6-tetramethyl-3,5-heptanedione with the Si(100)-2x1 surface: Scanning tunneling microscopy and density functional theory study. <i>Surface Science</i> , 2007, 601, 2887-2895.	0.8	15
2792	The absolute axial configurations of knipholone and knipholone anthrone by TDDFT and DFT/MRCI CD calculations: a revision. <i>Tetrahedron</i> , 2007, 63, 9810-9824.	1.0	30
2793	Theoretical study on the enantioselective α -amination reaction of 1,3-dicarbonyl compounds catalyzed by a bifunctional-urea. <i>Tetrahedron: Asymmetry</i> , 2007, 18, 1655-1662.	1.8	26
2794	A density functional theory study of the mechanism of the Paal-Knorr pyrrole synthesis. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 97-107.	1.5	30
2795	Solvent effects on ¹³ C and ¹ H NMR shielding of cyclic ketones: An experimental and theoretical study. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 203-213.	1.5	5
2796	DFT study of vibrational circular dichroism spectra of (S)-glycidol-water complexes. <i>Computational and Theoretical Chemistry</i> , 2007, 809, 161-169.	1.5	10
2797	Theoretical study of the reaction of Cu+ with OCS. <i>Computational and Theoretical Chemistry</i> , 2007, 810, 39-45.	1.5	2
2798	A computational investigation of the retrocyclization reaction of silacyclo-but-2-enes to 1-silabuta-1,3-dienes: Focus on the effect of the substituents. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 153-160.	1.5	8

#	ARTICLE	IF	CITATIONS
2799	The o-, m-, p-halobenzyl radicals and their anions: Structures and electron affinities. Computational and Theoretical Chemistry, 2007, 815, 45-53.	1.5	2
2800	DFT study of the substituent cross-interaction effects on the conformation of substituted N-benzylideneanilines – Models of liquid crystal forming compounds: Use of 13C NMR chemical shift of the CN Carbon as a tool to predict the conformation of the molecule. Computational and Theoretical Chemistry, 2007, 815, 95-104.	1.5	16
2801	A DFT study on the mechanism and regioselectivity of the tandem O-nitroso aldol/Michael reaction of nitrosobenzene and cyclohexenone. Computational and Theoretical Chemistry, 2007, 815, 105-109.	1.5	9
2802	Correlation of electrochemical and theoretical parameters in perylene diimide [60] fullerene dyads. Computational and Theoretical Chemistry, 2007, 815, 145-150.	1.5	8
2803	Structures and electron affinities of the halide (Cl, Br) benzene radicals. Computational and Theoretical Chemistry, 2007, 816, 67-72.	1.5	1
2804	Determination of precise harmonic force constants for alanine polypeptides. Computational and Theoretical Chemistry, 2007, 818, 125-129.	1.5	11
2805	Theoretical study on the aromaticity of dianions (X=Zn, Cd, Hg). Computational and Theoretical Chemistry, 2007, 818, 93-99.	1.5	33
2806	Theoretical probes of the host-guest complex: H-substituted cyclohexane encapsulated inside a self-assembled capsule. Computational and Theoretical Chemistry, 2007, 819, 153-159.	1.5	2
2807	Theoretical study of the reaction of Ni+ with OCS. Computational and Theoretical Chemistry, 2007, 820, 12-17.	1.5	7
2808	Theoretical mechanism for the oxidation of thiourea by hydrogen peroxide in gas state. Computational and Theoretical Chemistry, 2007, 821, 116-124.	1.5	5
2809	Performance of Time Dependent Density Functional Theory on excitations of medium sized molecules – Test on ionic forms of anthraquinone dihydroxy derivatives. Computational and Theoretical Chemistry, 2007, 823, 78-86.	1.5	28
2810	Structures and electron affinities of BrO2F and BrO3F. Chemical Physics Letters, 2007, 439, 395-401.	1.2	2
2811	Local hybrid exchange-correlation functionals based on the dimensionless density gradient. Chemical Physics Letters, 2007, 440, 160-168.	1.2	98
2812	A B3LYP study on the mechanism of second H2O formation in a fully reduced cytochrome c oxidase. Chemical Physics Letters, 2007, 440, 296-301.	1.2	7
2813	An indirect approach to the determination of the nuclear quadrupole moment by four-component relativistic DFT in molecular calculations. Chemical Physics Letters, 2007, 442, 233-237.	1.2	14
2814	Nuclear shielding constants from localized local hybrid exchange-correlation potentials. Chemical Physics Letters, 2007, 442, 496-503.	1.2	26
2815	Theoretical study on the mechanism of the Si_2 radical cation. Computational and Theoretical Chemistry, 2007, 823, 105-110.	1.2	8
2816	Ionic and neutral mercaptothiocarbonyl: A tandem mass spectrometry and computational study. Chemical Physics Letters, 2007, 443, 216-221.	1.2	6

#	ARTICLE	IF	CITATIONS
2817	Computational study of the reaction mechanism of benzylperoxy radical with HO ₂ in the gas phase. <i>Chemical Physics Letters</i> , 2007, 445, 17-21.	1.2	7
2818	Adsorption of CGA on colloidal silver particles: DFT and SERS study. <i>Chemical Physics Letters</i> , 2007, 444, 338-345.	1.2	89
2819	DFT calculations of NH ₃ adsorption and dissociation on gallium-rich GaAs(001)-4 \times 2 surface. <i>Chemical Physics Letters</i> , 2007, 445, 188-192.	1.2	7
2820	The electronic excited states of a model organic endoperoxide: A comparison of TD-DFT and ab initio methods. <i>Chemical Physics Letters</i> , 2007, 446, 262-267.	1.2	10
2821	Theoretical analysis of the electronic asymmetry of the special pair in the photosynthetic reaction center: Effect of structural asymmetry and protein environment. <i>Chemical Physics Letters</i> , 2007, 447, 324-329.	1.2	18
2822	Theoretical study of adsorption of gallium and gallium nitrides on Si(111). <i>Chemical Physics Letters</i> , 2007, 448, 88-92.	1.2	5
2823	Synthesis and conformational study of a new class of highly bioactive compounds. <i>Chemical Physics Letters</i> , 2007, 449, 336-340.	1.2	31
2824	A theoretical study of phenolic compounds with antioxidant properties. <i>European Journal of Medicinal Chemistry</i> , 2007, 42, 440-446.	2.6	46
2825	Comparative study of copper(II)-curcumin complexes as superoxide dismutase mimics and free radical scavengers. <i>European Journal of Medicinal Chemistry</i> , 2007, 42, 431-439.	2.6	151
2826	Morphology and structure of poly(p-dioxanone). <i>European Polymer Journal</i> , 2007, 43, 4662-4674.	2.6	20
2827	Geometries and properties of bimetallic phosphido-bridged complex Cp(CO) ₂ W(η -PPh ₂)W(CO) ₅ and Cp(CO) ₃ W(η -PPh ₂)W(CO) ₅ . <i>Chemical Physics</i> , 2007, 332, 33-38.	0.9	1
2828	Explicit role of dynamical and nondynamical electron correlation on singlet-triplet splitting in carbenes. <i>Chemical Physics</i> , 2007, 332, 232-242.	0.9	4
2829	Proton and hydrogen atom adducts to cytosine. An experimental and computational study. <i>International Journal of Mass Spectrometry</i> , 2007, 265, 106-123.	0.7	33
2830	Cytosine neutral molecules and cation-radicals in the gas-phase. <i>International Journal of Mass Spectrometry</i> , 2007, 267, 30-42.	0.7	61
2831	Cyano substituent effects on enol and enethiol acidity and basicity: The protonation and deprotonation of 3-hydroxy-2-propenenitrile and its thio analogue. <i>International Journal of Mass Spectrometry</i> , 2007, 267, 125-133.	0.7	18
2832	C ₂ H ₂ S radical cations: Application of tandem mass spectrometry methodologies. <i>International Journal of Mass Spectrometry</i> , 2007, 263, 289-297.	0.7	16
2833	Vibrational spectra of oligothieryl-vinylenes with donor-acceptor and donor-acceptor substitution patterns. <i>Journal of Molecular Structure</i> , 2007, 834-836, 374-379.	1.8	1
2834	Gaseous nitril azide N ₄ O ₂ : A joint theoretical and experimental study. <i>Journal of Molecular Structure</i> , 2007, 840, 59-65.	1.8	12

#	ARTICLE	IF	CITATIONS
2835	Vibrational spectra of nonlinear optical chromophores based on octopolar C ₃ -symmetric 1,3,5 trisubstituted benzenes. <i>Journal of Molecular Structure</i> , 2007, 834-836, 369-373.	1.8	2
2836	Electron localization function (ELF) study on intramolecular delocalization of the electron density in the H ₂ X, H ₂ CX and XO ₂ (X=O, S, Se, Te) molecules: Role of the atomic core and lone pair. <i>Journal of Molecular Structure</i> , 2007, 844-845, 278-285.	1.8	7
2837	Activation of light alkanes over Cd ²⁺ ions in ZSM-5 zeolite: a theoretical study. <i>Mendeleev Communications</i> , 2007, 17, 68-70.	0.6	8
2838	Electronic spectroscopy study and molecular docking simulation of the interaction of terthiophene with DNA. <i>Journal of Molecular Structure</i> , 2007, 834-836, 176-181.	1.8	4
2839	A methylenic group binds guanidinoacetic acid to glycine and serine in two novel copper(II) complexes: Synthesis, X-ray structure and spectroscopic characterization. <i>Polyhedron</i> , 2007, 26, 4363-4372.	1.0	8
2840	Effects of the ancillary ligands of polypyridyl ruthenium(II) complexes on the DNA-binding and photocleavage behaviors. <i>Polyhedron</i> , 2007, 26, 5458-5468.	1.0	49
2841	A theoretical study on the interaction between N-methylpyrrole and 3,4-ethylenedioxythiophene units in copolymer molecules. <i>Polymer</i> , 2007, 48, 6162-6169.	1.8	3
2842	On the structural and electronic properties of poly(3-thiophen-3-yl-acrylic acid methyl ester). <i>Polymer</i> , 2007, 48, 6955-6964.	1.8	18
2843	A DFT/TDDFT study on the structures, trend in DNA-binding and spectral properties of molecular "light switch" complexes [Ru(phen) ₂ (L)] ²⁺ (L=dppz, taptp, phehat). <i>Journal of Organometallic Chemistry</i> , 2007, 692, 831-838.	0.8	32
2844	Reactivity of TpRu(L)(NCMe)R (L=CO, PMe ₃ ; R=Me, Ph) systems with isonitriles: Experimental and computational studies toward the intra- and intermolecular hydroarylation of isonitriles. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 2175-2186.	0.8	15
2845	Spin density distribution in mononuclear Rh(0) complexes: A combined experimental and DFT study. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 3167-3173.	0.8	20
2846	Hydrogen sensitivity "A systematic computational study of electronic effects. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 4473-4480.	0.8	6
2847	Computational study of methane functionalization by a multiply bonded, Ni-bis(phosphine) complex. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 4551-4559.	0.8	18
2848	Bis(η ⁵ -cyclopentadienyl)titanium(II) in the gas phase. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 4073-4083.	0.8	11
2849	A possible 2,1→3,1 isomerization mechanism in zirconocene-catalyzed propene polymerization: An application of the density functional theory and combined ONIOM approach. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 4227-4236.	0.8	12
2850	Synthesis and crystal structures of the first C ₂ -symmetric bis-aldimine NCN "pincer" complexes of platinum and palladium. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 4843-4848.	0.8	37
2851	Synthesis of ferrocenyl pyrazoles by the reaction of (2-formyl-1-chlorovinyl)ferrocene with hydrazines. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 5026-5032.	0.8	53
2852	Theoretical study on electronic structures of FeOO, FeOOH, FeO(H ₂ O), and FeO in hemes: As intermediate models of dioxygen reduction in cytochrome c oxidase. <i>Journal of Inorganic Biochemistry</i> , 2007, 101, 1410-1427.	1.5	24

#	ARTICLE	IF	CITATIONS
2853	Vibrational spectra and assignments of 5-amino-2-chlorobenzoic acid by ab initio Hartree-Fock and density functional methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 66, 381-388.	2.0	49
2854	FT-IR vibrational spectrum and DFT:B3LYP/6-31G structure and vibrational analysis of guanidinoaceticserinenickel(II) complex: [Ni(GAA)(Ser)]. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 67, 1037-1045.	2.0	18
2855	FT-IR vibrational spectrum and DFT:B3LYP/6-311G structure and vibrational analysis of bis-serinenickel(II) complex: [Ni(Ser) ₂]. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 67, 1046-1054.	2.0	12
2856	Fourier transform infrared spectrum, vibrational analysis and structural determinations of the trans-bis(glycine)nickel(II) complex by means of the RHF/6-311G and DFT:B3LYP/6-31G and 6-311G methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 68, 1370-1378.	2.0	35
2857	Electron capture in spin-trap capped peptides. An experimental example of ergodic dissociation in peptide cation-radicals. <i>Journal of the American Society for Mass Spectrometry</i> , 2007, 18, 432-444.	1.2	37
2858	Vanadia-based SCR catalysts supported on tungstated and sulfated zirconia: Influence of doping with potassium. <i>Journal of Catalysis</i> , 2007, 251, 459-473.	3.1	91
2859	Growth of ZrC thin films by aerosol-assisted MOCVD. <i>Journal of Crystal Growth</i> , 2007, 304, 324-332.	0.7	44
2860	Experimental and theoretical investigation of the pH effect on the titania phase transformation during the sol-gel process. <i>Journal of Crystal Growth</i> , 2007, 308, 122-129.	0.7	38
2861	Analysis of self-interaction correction for describing core excited states. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 23-29.	1.0	43
2862	Ab initio quantum chemical studies of the reactions of CF ₃ CFHO ₂ with HO ₂ . <i>International Journal of Quantum Chemistry</i> , 2007, 107, 46-55.	1.0	6
2863	Theoretical study of aromaticity in small hydrogen and metal cation clusters X ₃ (X=H, Li, Na, K, and) Tj ETQq0 0 0 rBT /Overlock 10 Tf	1.0	30
2864	Modeling the cyclopolymerization of diallyl ether and methyl $\hat{\pm}$ -[(allyloxy)methyl]acrylate. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 894-906.	1.0	9
2865	Conformational analysis and the binding sites of nitrilotriacetamide: A computational study. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1430-1436.	1.0	1
2866	DFT-based QSAR study and molecular design of AHMA derivatives as potent anticancer agents. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1468-1478.	1.0	20
2867	Swift hopping gallium over [AlO ₄] ⁻ tetrahedra in Ga/ZSM-5: A DFT study. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2434-2441.	1.0	5
2868	Reaction-path dynamics and theoretical rate constants for the reaction CH ₄ + O ₃ $\hat{\pm}$ ' HOOO + CH ₃ . <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1999-2005.	1.0	14
2869	A force field for simulating ethanol adsorption on Au(111) surfaces. A DFT study. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2169-2177.	1.0	20
2870	Density functional study of manganese dimer. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3178-3190.	1.0	21

#	ARTICLE	IF	CITATIONS
2871	Hybrid density functional study of ligand coordination effects on the magnetic couplings and the dioxygen binding of the models of hemocyanin. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3103-3119.	1.0	16
2872	A computational study into the reactivity of epichlorohydrin and epibromohydrin under basic conditions in the gas phase and solution. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 19-29.	0.9	7
2873	Brotherversusbrother: competitive stabilization of carbocationic centers by flanking cyclopropanes and π -systems. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 384-394.	0.9	10
2874	Structure and properties of β -cyclo[N]thiophenes as potential electronic materials - a theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 554-567.	0.9	19
2875	Initiation of petroleum formation and antioxidant function - a DFT study of sulfur-sulfur bond dissociation enthalpies. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 754-763.	0.9	4
2876	Adsorption properties of oxidized gallium-modified zeolite ZSM-5 from diffuse reflectance IR and quantum-chemical data: 1. Interaction with hydrogen and ethane. <i>Kinetics and Catalysis</i> , 2007, 48, 735-741.	0.3	4
2877	Reaction of PtCl ₄ with 18-crown-6 in aprotic solvents (Nitromethane, acetonitrile, and Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50,502 Td (1,	0.3	3
2878	Coherent signal amplification in rhodopsin media. <i>Physics of Particles and Nuclei Letters</i> , 2007, 4, 150-153.	0.1	1
2879	Oligothiophene- and Oligopyrrole-Mediated Aggregation of Gold Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2007, 111, 5886-5892.	1.5	18
2880	Origin of the different emission wavelengths in Alq ₃ analyzed by solid-state NMR. <i>Proceedings of SPIE</i> , 2007, , .	0.8	0
2881	Generation of Free Radicals by Emodic Acid and its [d-Lys6]GnRH-conjugate. <i>Photochemistry and Photobiology</i> , 2007, 74, 226-236.	1.3	1
2882	The aluminum arsenides AlMAsn (mâ€™%+â€™%nâ€™%â€™%2â€™%5) and their anions: Structures, electron affinities and vibrational frequencies. <i>European Physical Journal D</i> , 2007, 42, 259-267.	0.6	9
2883	Probing the structural effects on the intrinsic electronic and redox properties of [2Feâ€™2S] ⁺ clusters, a broken-symmetry density functional theory study. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 275-281.	0.5	11
2884	Electronic structures of 4d transition metal monoxides by density functional theory. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 407-415.	0.5	40
2885	A test case for time-dependent density functional theory calculations of electronic circular dichroism: 2-chloro-4-methoxy-6- [(R)-1-phenylethylamino]-1,3,5- triazine. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 793-803.	0.5	1
2886	Effects of protonation on proton transfer processes in Watsonâ€™Crick adenineâ€™thymine base pair. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 113-121.	0.5	36
2887	A barrier-free molecular radical-molecule reaction: $\text{C}_2^+ (\text{a}^3\Pi) + \text{O}_2 (\text{X}^3\Sigma^-)$ Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 102	0.5	3
2888	New computational evidence for the catalytic mechanism of carbonic anhydrase. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 193-201.	0.5	41

#	ARTICLE	IF	CITATIONS
2889	A tunable QM/MM approach to chemical reactivity, structure and physico-chemical properties prediction. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 219-240.	0.5	86
2890	Reparameterization of a meta-generalized gradient approximation functional by combining TPSS exchange with I_{H} correlation. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 693-707.	0.5	19
2891	In search of 1,3-disila/germa/stannabicyclo[1.1.1]pentanes with short bridgehead-bridgehead distances and low ring strain energies. <i>Silicon Chemistry</i> , 2007, 3, 165-173.	0.8	2
2892	X-ray structural analyses and DFT study of 7-thianorbornenes: 4-aza-4-phenyl-10-thiatricyclo[5.2.1.0.2,6]deca-8-ene-3,5-dione and 4-aza-1,4,7-trimethyl-10-thiatricyclo[5.2.1.0.2,6]deca-8-ene-3,5-dione. <i>Structural Chemistry</i> , 2007, 18, 279-286.	1.0	4
2893	Mild template synthesis of copper(II)-containing macrocyclic compounds in the Cull ²⁺ -1,2-diaminoethanedithione-1,2 ²⁻ -ethanedione-1,2 and Cull ²⁺ -1,2-diamino-ethanedithione-1,2 ²⁻ -butanedione-2,3 triple systems into Cu ₂ [Fe(CN) ₆]-gelatin-immobilized matrix implantates. <i>Transition Metal Chemistry</i> , 2007, 32, 1056-1060.	0.7	7
2894	Hybrid exchange correlation functionals and potentials: Concept elaboration. <i>Journal of Structural Chemistry</i> , 2007, 48, S1-S31.	0.3	40
2895	Chromium(III) Hydroxide Solubility in the Aqueous $K^+ + H^+ + OH^{2-} + CO_2 + HCO_3^- + CO_3^{2-} + H_2O$ System: A Thermodynamic Model. <i>Journal of Solution Chemistry</i> , 2007, 36, 1261-1285.	0.6	43
2896	Systematic study on the mechanism of aldehyde oxidation to carboxylic acid by cytochrome P450. <i>Journal of Biological Inorganic Chemistry</i> , 2007, 12, 1073-1081.	1.1	17
2897	Theoretical study of the catalytic mechanism of catechol oxidase. <i>Journal of Biological Inorganic Chemistry</i> , 2007, 12, 1251-1264.	1.1	37
2898	Theoretical study of N ₄ X (X = O, S, Se) systems. <i>Journal of Molecular Modeling</i> , 2007, 13, 1073-1080.	0.8	4
2899	A comparison of transition state of phenol in H-atom abstraction by methyl and methylperoxyl radicals. <i>Science Bulletin</i> , 2007, 52, 1182-1186.	1.7	2
2900	Reactivity of tourmaline by quantum chemical calculations. <i>Journal Wuhan University of Technology, Materials Science Edition</i> , 2007, 22, 673-676.	0.4	2
2901	Complexes of dichloro(ethylenediamine)palladium(II) observed from aqueous solutions by electrospray mass spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2007, 18, 769-777.	1.2	9
2902	Electron capture in charge-tagged peptides. Evidence for the role of excited electronic states. <i>Journal of the American Society for Mass Spectrometry</i> , 2007, 18, 2146-2161.	1.2	58
2903	Assessment of density-functional models for organic molecular semiconductors: The role of Hartree-Fock exchange in charge-transfer processes. <i>Chemical Physics</i> , 2007, 331, 321-331.	0.9	63
2904	Comparison of theoretical approaches for computing the bond length alternation of polymethineimine. <i>Chemical Physics</i> , 2007, 332, 79-85.	0.9	22
2905	Direct dynamics study on hydrogen abstraction reaction of CF ₃ CHOHCF ₃ with OH radical. <i>Chemical Physics</i> , 2007, 335, 28-36.	0.9	4
2906	Modelling water adsorption on Au(210) surfaces. I. A force field for water ²⁺ -Au interactions by DFT. <i>Journal of Electroanalytical Chemistry</i> , 2007, 609, 140-146.	1.9	20

#	ARTICLE	IF	CITATIONS
2907	The photophysics of 7H-adenine: A quantum chemical investigation including spin-orbit effects. <i>Chemical Physics</i> , 2008, 347, 346-359.	0.9	23
2908	Inverse hydrogen migration in arginine-containing peptide ions upon electron transfer. <i>Journal of the American Society for Mass Spectrometry</i> , 2008, 19, 1726-1742.	1.2	30
2909	Structural and electronic properties of poly(3-thiophen-3-yl-acrylic acid). <i>Polymer</i> , 2008, 49, 1972-1980.	1.8	12
2910	Synthesis and rhodium complexation of enantiomerically enriched bicyclo[3.3.1]nona-2,6-diene. <i>Tetrahedron: Asymmetry</i> , 2008, 19, 1328-1332.	1.8	16
2911	Theoretical study on the oxidation mechanism of thiourea by hydrogen peroxide with water and hydroxyl assistance. <i>Computational and Theoretical Chemistry</i> , 2008, 850, 121-126.	1.5	3
2912	Static first order hyperpolarizabilities of DNA base pairs: A configuration interaction study. <i>Computational and Theoretical Chemistry</i> , 2008, 855, 64-68.	1.5	12
2913	Computational study on dipole moment, polarizability and second hyperpolarizability of nitronaphthalenes. <i>Computational and Theoretical Chemistry</i> , 2008, 856, 105-111.	1.5	20
2914	Structure and stability of thioureate anions with water, DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2008, 858, 101-106.	1.5	3
2915	DFT modelling of cobalt and nickel complexes with dithiophosphinic acid. <i>Computational and Theoretical Chemistry</i> , 2008, 859, 93-97.	1.5	10
2916	The selenium oxygen clusters SeOn (n=1-5) and their anions: Structures and electron affinities. <i>Computational and Theoretical Chemistry</i> , 2008, 863, 1-8.	1.5	10
2917	A theoretical study on the gas phase reaction of Pd+ and Pt+ with CS2. <i>Computational and Theoretical Chemistry</i> , 2008, 867, 85-89.	1.5	2
2918	Soft template synthesis in the cobalt(III)-1,2-diaminoethane-1,2-dithione-propanone triple system on a K[CoFe(CN)6]-gelatin-immobilized matrix. <i>Transition Metal Chemistry</i> , 2008, 33, 523-527.	0.7	7
2919	Structures, Mechanisms, and Kinetics of Selective Ammoxidation and Oxidation of Propane over Multi-metal Oxide Catalysts. <i>Topics in Catalysis</i> , 2008, 50, 2-18.	1.3	56
2920	Effect of local sugar and base geometry on 13C and 15N magnetic shielding anisotropy in DNA nucleosides. <i>Journal of Biomolecular NMR</i> , 2008, 42, 209-223.	1.6	7
2921	Coordination Features of Polyaza-Bipyridine-Macrocyclic Ligand toward Co(II) and Cd(II) in Water and Dimethylsulfoxide. <i>Journal of Solution Chemistry</i> , 2008, 37, 503-517.	0.6	9
2922	Environmental Mobility of Pu(IV) in the Presence of Ethylenediaminetetraacetic Acid: Myth or Reality?. <i>Journal of Solution Chemistry</i> , 2008, 37, 957-986.	0.6	19
2923	Thermodynamic Model for ThO2(am) Solubility in Alkaline-Silica Solutions. <i>Journal of Solution Chemistry</i> , 2008, 37, 1725-1746.	0.6	12
2924	An IEF-PCM study of solvent effects on the Faraday B term of MCD. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 231-244.	0.5	31

#	ARTICLE	IF	CITATIONS
2925	Kinetics of the hydrogen abstraction CHO + Alkane → HCHO + Alkyl reaction class: an application of the reaction class transition state theory. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 107-118.	0.5	10
2926	A theoretical study of the reaction of Ti ⁺ with propane. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 243-261.	0.5	9
2927	Theoretical design of blue emitting materials based on symmetric and asymmetric spiro-silabifluorene derivatives. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 489-500.	0.5	12
2928	Technical aspects of quantum chemical modeling of enzymatic reactions: the case of phosphotriesterase. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 515-522.	0.5	67
2929	Theoretical investigation of the catalytic mechanism of the protein arginine deiminase 4 enzyme. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 459-466.	0.5	13
2930	Theoretical study of the biologically important dioxo diiron diamond core structures. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 467-478.	0.5	2
2931	Theoretical study of the reaction of ethynyl radical with acetonitrile. <i>Theoretical Chemistry Accounts</i> , 2008, 121, 33-41.	0.5	4
2932	End-substitution effect on the geometry and electronic structure of oligoheterocyclics. <i>Theoretical Chemistry Accounts</i> , 2008, 121, 109-122.	0.5	9
2933	A QSAR study and molecular design of benzothiazole derivatives as potent anticancer agents. <i>Science in China Series B: Chemistry</i> , 2008, 51, 111-119.	0.8	10
2934	Electronic properties of some nitrobenzo[a]pyrene isomers: a possible relationship to mutagenic activity. <i>Journal of Molecular Modeling</i> , 2008, 14, 489-497.	0.8	16
2935	Improved electrostatic properties using combined Mulliken and hybridization-displaced charges for radicals. <i>Journal of Molecular Modeling</i> , 2008, 14, 631-640.	0.8	9
2936	Theoretical and experimental study of molecular structure and vibrational spectra of N-(2-pyridylmethyl)-2-pyrazinecarboxamide. <i>Monatshefte für Chemie</i> , 2008, 139, 773-780.	0.9	19
2937	Electronic effects of heterocyclic ring systems as evaluated with the aid of ¹³ C and ¹⁵ N NMR chemical shifts and NBO analysis. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 173-184.	0.9	15
2938	Structural aspects of the intermolecular hydrogen bond strength: H-bonded complexes of aniline, phenol and pyridine derivatives. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 897-914.	0.9	80
2939	The oxidation of alcohols to aldehydes and ketones with N-bromosuccinimide in polyethylene glycol: an experimental and theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 945-953.	0.9	20
2940	DFT study of the biphenylene-NO complexes formed in nitration mechanism. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 971-978.	0.9	10
2941	Mass spectra of tetrahydroisoquinoline-fused 1,3,2-oxazapine and 1,2,3-oxazapine heterocycles: influence of ring size and fusion, of present heteroatoms, substituent effects and of the stereochemistry on fragmentation. <i>Rapid Communications in Mass Spectrometry</i> , 2008, 22, 1519-1527.	0.7	4
2942	Growth mechanism of catalyst- and template-free InN nanorods. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2008, 5, 1633-1638.	0.8	3

#	ARTICLE	IF	CITATIONS
2943	Accurate and Validated Quantitative Structure–Activity Relationship Model of Caspase–Mediated Apoptosis–Inducing Activity of Phenolic Compounds Using Density Functional Theory Calculation and Genetic Algorithm–Multiple Linear Regression. <i>QSAR and Combinatorial Science</i> , 2008, 27, 1318-1325.	1.5	4
2944	Poor enantioselectivity of the direct aldol reaction catalyzed by (S,S)-proline dipeptide: A density functional study. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 66-74.	1.0	2
2945	Harmonic force field for glycine oligopeptides. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 180-188.	1.0	18
2946	Theoretical study of ignition reactions of linear symmetrical monoethers as potential diesel fuel additives: DFT calculations. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 40-50.	1.0	7
2947	Ab initio reaction path for cisplatin interaction with L-cysteine and L-methionine. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 401-414.	1.0	19
2948	Improving the TDDFT calculation of low-lying excited states for polycyclic aromatic hydrocarbons using the Tamm–Dancoff approximation. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 430-439.	1.0	62
2949	A barrier-free atomic radical–molecule reaction: N(² D) NO(₂) (² A ₁) mechanistic study. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1309-1315.	1.0	2
2950	DFT study for the reactions of H atoms with CH ₃ OH and C ₂ H ₅ OH. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2476-2485.	1.0	18
2951	Effects of substituents on molecular devices. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1546-1554.	1.0	14
2952	On the binding mode of urease active site inhibitors: A density functional study. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2023-2029.	1.0	8
2953	The hybrid–DFT study on bandgap estimation for the perovskite-type titanium oxide of SrTiO ₃ . <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2856-2861.	1.0	23
2954	Exciting prospects for solids: Exact–exchange based functionals meet quasiparticle energy calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 929-945.	0.7	83
2955	Ni ⁺ reactions with aminoacetonitrile, a potential prebiological precursor of glycine. <i>Journal of Mass Spectrometry</i> , 2008, 43, 317-326.	0.7	9
2956	Xylogranatins F: Antifeedants from the Chinese Mangrove, <i>Xylocarpus granatum</i> , A New Biogenetic Pathway to Tetranortriterpenoids. <i>Chemistry - A European Journal</i> , 2008, 14, 1129-1144.	1.7	81
2957	Energetics and Mechanism of Ammonia Synthesis through the Chatt Cycle: Conditions for a Catalytic Mode and Comparison with the Schrock Cycle. <i>Chemistry - A European Journal</i> , 2008, 14, 644-652.	1.7	77
2958	Modeling the Photochemistry of the Reference Phototoxic Drug Lomefloxacin by Steady-State and Time-Resolved Experiments, and DFT and Post-HF Calculations. <i>Chemistry - A European Journal</i> , 2008, 14, 653-663.	1.7	43
2959	Switchable C- and N-Bound Isomers of Transition-Metal Cyanocarbanions: Synthesis and Interconversions of Cyclopentadienyl Ruthenium Complexes of Phenylsulfonylacetonitrile Anions. <i>Chemistry - A European Journal</i> , 2008, 14, 2482-2498.	1.7	17
2960	Density Functional Theory Study of <i>trans</i> -Dioxo Complexes of Iron, Ruthenium, and Osmium with Saturated Amine Ligands, <i>trans</i> -[M(O) ₂ (NH ₃) ₂ (NMeH ₂) ₂] ^{2±} (M=Fe, Ru, Os), and Detection of [Fe(qpy)(O) ₂] ⁺ (<i>n</i> =1, 2) by High-Resolution ESI Mass Spectrometry. <i>Chemistry - A European Journal</i> , 2008, 14, 5495-5506.		13

#	ARTICLE	IF	CITATIONS
2961	Bonding in Tropolone, 2-aminotropone, and aminotroponimine: No Evidence of Resonance-Assisted Hydrogen-Bond Effects. <i>Chemistry - A European Journal</i> , 2008, 14, 4225-4232.	1.7	80
2962	A Rigid, Chiral, Dendronized Polymer with a Thermally Stable, Right-Handed Helical Conformation. <i>Chemistry - A European Journal</i> , 2008, 14, 6924-6934.	1.7	49
2963	Magnetic Endohedral Transition-Metal-Doped Semiconducting Nanoclusters. <i>Chemistry - A European Journal</i> , 2008, 14, 8547-8554.	1.7	10
2964	Coordination Chemistry of Conformationally Flexible 1,2,3,4,5,6-Cyclohexanhexacarboxylate: Trapping Various Conformations in Metal-Organic Frameworks. <i>Chemistry - A European Journal</i> , 2008, 14, 7218-7235.	1.7	72
2965	Mechanisms of Air Oxidation of Ethoxylated Surfactants—Computational Estimations of Energies and Reaction Behaviors. <i>Chemistry - A European Journal</i> , 2008, 14, 9549-9554.	1.7	8
2966	Reaction Mechanism of Molybdoenzyme Formate Dehydrogenase. <i>Chemistry - A European Journal</i> , 2008, 14, 8674-8681.	1.7	47
2967	\hat{I}_1, \hat{I}_2 -Unsaturated and Saturated Derivatives of Be, Mg, and Ca: Are They Carbon or Metal Acids in the Gas Phase?. <i>Chemistry - A European Journal</i> , 2008, 14, 10423-10429.	1.7	8
2968	Predicting Reactivity and Stereoselectivity in the Nazarov Reaction: A Combined Computational and Experimental Study. <i>Chemistry - A European Journal</i> , 2008, 14, 9292-9304.	1.7	27
2969	New β -Spiro Ladder-Type Phenylene Materials: Synthesis, Physicochemical Properties and Applications in OLEDs. <i>Chemistry - A European Journal</i> , 2008, 14, 11328-11342.	1.7	73
2970	Intervalent Bis(η^4 -aziridinato) $M^{II}M^I$ Complexes (M=Rh, Ir): Delocalized Metallo-Radicals or Delocalized Aminyl Radicals?. <i>Chemistry - A European Journal</i> , 2008, 14, 10985-10998.	1.7	10
2971	Measured and calculated CD spectra of G-quartets stacked with the same or opposite polarities. <i>Chirality</i> , 2008, 20, 431-440.	1.3	202
2972	Theoretical insight into the influences of \hat{I}_1 -substituents in aliphatic aldehydes on the enantioselectivities of aldol reactions. <i>Chirality</i> , 2008, 20, 54-61.	1.3	4
2973	δ -Thioguanine in DNA as CD spectroscopic probe to study local structural changes upon protein binding. <i>Chirality</i> , 2008, 20, 978-984.	1.3	8
2974	Calculation of conformational energies and optical rotation of the most simple chiral alkane. <i>Chirality</i> , 2008, 20, 1009-1015.	1.3	33
2975	Hydrogen Atom Release Dynamics in Radical-Initiated Radical Reactions: Saturated vs Unsaturated. <i>ChemPhysChem</i> , 2008, 9, 1099-1103.	1.0	6
2976	Theoretical Investigation of the OH-Initiated Oxidation of Benzaldehyde in the Troposphere. <i>ChemPhysChem</i> , 2008, 9, 1453-1459.	1.0	19
2977	Tunneling Splittings in the S_0 and S_1 States of the Benzoic Acid Dimer Determined by High-Resolution UV Spectroscopy. <i>ChemPhysChem</i> , 2008, 9, 1788-1797.	1.0	44
2978	Why Are Selenouracils as Basic as but Stronger Acids than Uracil in the Gas Phase?. <i>ChemPhysChem</i> , 2008, 9, 1715-1720.	1.0	5

#	ARTICLE	IF	CITATIONS
2979	Synthesis, DNA-Binding and Photocleavage Studies of the Ruthenium(II) Complexes [Ru(phen) ₂ (ppd)] ²⁺ and [Ru(phen)(ppd) ₂] ²⁺ (ppd=Peridino[6,7-f]-%[1,10]phenanthroline-1,13(10-H,12-H)-dione.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.0	24
2980	Experimental and Theoretical Studies on DNA-Binding and Spectral Properties of "Light Switch"™ Complexes [Ru(L) ₂ (ppn)] ²⁺ (L=2,2'-Bipyridine and 1,10-Phenanthroline;) Tj ETQq1.0 0.784314 rgBT /	1.0	14
2981	Benchmarking approximate density functional theory for s/d excitation energies in 3d transition metal cations. Journal of Computational Chemistry, 2008, 29, 185-189.	1.5	61
2982	Direct dynamics study on the reaction of acetaldehyde with ozone. Journal of Computational Chemistry, 2008, 29, 247-255.	1.5	10
2983	Torsional effects on excitation energies of thiophene derivatives induced by ² substituents: Comparison between time-dependent density functional theory and approximated coupled cluster approaches. Journal of Computational Chemistry, 2008, 29, 451-457.	1.5	11
2984	Theoretical study of the reactions CF ₃ CH ₂ OCHF ₂ + OH/Cl and its product radicals and parent ether(CH ₃ CH ₂ OCH ₃) with OH. Journal of Computational Chemistry, 2008, 29, 550-561.	1.5	26
2985	Calculation of weakly polar interaction energies in polypeptides using density functional and local MÅller-Plesset perturbation theory. Journal of Computational Chemistry, 2008, 29, 1344-1352.	1.5	30
2986	Theoretical study on the structure and formation mechanism of [C ₆ H ₅ M<i>m</i>] ⁺ (M=3/4Ag, Au; <i>m</i> = 1-3). Journal of Computational Chemistry, 2008, 29, 1667-1674.	1.5	10
2987	Theoretical investigation of anthracene-9,10-endoperoxide vertical singlet and triplet excitation spectra. Journal of Computational Chemistry, 2008, 29, 1982-1991.	1.5	15
2988	Stereoelectronic properties of spiroquinazolinones in differential PDE7 inhibitory activity. Journal of Computational Chemistry, 2008, 29, 1945-1954.	1.5	25
2989	Application of the Sakurai-Sugiura projection method to core-excited state calculation by time-dependent density functional theory. Journal of Computational Chemistry, 2008, 29, 2311-2316.	1.5	21
2990	<i>Ab-initio</i> simulations of materials using VASP: Density-functional theory and beyond. Journal of Computational Chemistry, 2008, 29, 2044-2078.	1.5	2,717
2991	Synthesis, Crystal Structure and Thermal Reactivity of [ZnX ₂](2-chloropyrazine)] (X = Cl,) Tj ETQq0 0 0 rgBT /Overlock 10	1.0	14
2992	Aminopyrimidine-Based Donor-Acceptor Chromophores: Push-Pull versus Aromatic Behaviour. European Journal of Organic Chemistry, 2008, 2008, 99-108.	1.2	25
2993	Synthesis and Conformational Analysis of Tetrahydroisoquinoline-Fused 1,3,2-Oxazaphospholidines and 1,2,3-Oxathiazolidines. European Journal of Organic Chemistry, 2008, 2008, 1464-1472.	1.2	8
2994	Nucleohomolytic Substitution at Boron: A Computational Approach. European Journal of Organic Chemistry, 2008, 2008, 4454-4459.	1.2	24
2995	Boron-Based Diastereomerism and Enantiomerism in Imine Complexes " Determination of the Absolute Configuration at Boron by CD Spectroscopy. European Journal of Organic Chemistry, 2008, 2008, 5221-5225.	1.2	25
2996	Neutral MÅrbius Aromatics: Derivatives of the Pyrrole Congener Aza[11]annulene as Promising Synthetic Targets. European Journal of Organic Chemistry, 2008, 2008, 5755-5763.	1.2	11

#	ARTICLE	IF	CITATIONS
2997	The role of weakly polar and Hâ€bonding interactions in the stabilization of the conformers of FGG, WGG, and YGG; An aqueous phase computational study. <i>Biopolymers</i> , 2008, 89, 1002-1011.	1.2	6
2998	A Polar Radical Pair Pathway To Assemble the Pyrimidinone Core of the HIV Integrase Inhibitor Raltegravir Potassium. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 4134-4136.	7.2	25
2999	Pronounced Steric Effects of Substituents in the Nazarov Cyclization of Aryl Dienyl Ketones. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 6379-6383.	7.2	67
3000	Is Allred's [Hg(cyclam)] ³⁺ a True Mercury(III) Complex?. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 8631-8633.	7.2	18
3001	Gasâ€Phase Formation of the Gombergâ€Bachmann Magnesium Ketyl. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 9118-9121.	7.2	38
3002	Oligophenylenevinylenes in Spatially Confined Nanochannels: Monitoring Intermolecular Interactions by UV/Vis and Raman Spectroscopy. <i>Advanced Functional Materials</i> , 2008, 18, 915-921.	7.8	20
3003	The Cycloaddition Reaction Between Î±-Bromo Vinylketenes and Imines: A Combined Experimental and Theoretical Study. <i>Advanced Synthesis and Catalysis</i> , 2008, 350, 2261-2273.	2.1	5
3008	Quantitative aspects of and ionization mechanisms in positive-ion atmospheric pressure chemical ionization mass spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2008, 19, 1926-1941.	1.2	40
3009	Growth mechanism of catalyst- and template-free group III-nitride nanorods. <i>Journal of Crystal Growth</i> , 2008, 310, 3735-3740.	0.7	14
3010	Synthesis, characterization and crystal structure determination of zinc (II) and mercury (II) complexes with 2,2'-dimethyl-4,4'-bithiazole. <i>Polyhedron</i> , 2008, 27, 1848-1854.	1.0	51
3011	An integrated experimental and theoretical investigation of the vibrational modes and molecular structure of a new Cu(II)-phosphocreatine complex. <i>Polyhedron</i> , 2008, 27, 3662-3668.	1.0	7
3012	On the molecular properties of polyaniline: A comprehensive theoretical study. <i>Polymer</i> , 2008, 49, 5169-5176.	1.8	53
3013	Structural and spectroscopic study of the Br ²⁺ -Br-pyridine complex by DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 69, 933-938.	2.0	2
3014	FT-IR, FT-Raman spectra and quantum chemical calculations of 3,4-dimethoxyaniline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 70, 50-59.	2.0	18
3015	Vibrational spectra and quantum chemical calculations of 3,4-diaminobenzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 70, 376-383.	2.0	33
3016	FT-IR, FT-Raman spectra and ab initio HF and DFT calculations of 4-N,N'-dimethylamino pyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 898-906.	2.0	144
3017	Theoretical surface-enhanced Raman spectra study of substituted benzenes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1049-1055.	2.0	34
3018	Theoretical surface-enhanced Raman spectra study of substituted benzenes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1074-1079.	2.0	15

#	ARTICLE	IF	CITATIONS
3019	Vibrational spectra and structure of isopropylbenzene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1128-1133.	2.0	3
3020	Molecular structure and vibrational spectra of 3-chloro-4-fluoro benzonitrile by ab initio HF and density functional method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1134-1139.	2.0	80
3021	Experimental and density functional theory (DFT) studies on the DNA-binding trend and spectral properties of two new Ru(II) complexes: [Ru(L)2(mip)](ClO4)2 (L=2,9-dmp and 4,7-dmp). <i>Journal of Organometallic Chemistry</i> , 2008, 693, 3387-3395.	0.8	17
3022	Disilane- and siloxane-bridged biphenyl and bithiophene derivatives as electron-transporting materials in OLEDs. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 3490-3494.	0.8	32
3023	Theoretical study on the consecutive 1,2-hydroboration and 1,1-organoboration reactions of alkyn-1-yl(vinyl)silane with borane. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 3722-3728.	0.8	9
3024	Theoretical investigation of the photosensitization mechanisms of urocanic acid. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2008, 91, 96-98.	1.7	11
3025	A theoretical study on the quenching mechanisms of triplet state riboflavin by tryptophan and tyrosine. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2008, 92, 10-12.	1.7	12
3026	The photophysics of flavins: What makes the difference between gas phase and aqueous solution?. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2008, 198, 221-231.	2.0	93
3027	Mapping Potential Energy Surfaces by Neural Networks: The ethanol/Au(111) interface. <i>Journal of Electroanalytical Chemistry</i> , 2008, 624, 109-120.	1.9	20
3028	Prediction of mutagenic activity of nitronaphthalene isomers by infrared and Raman spectroscopy. <i>Journal of Hazardous Materials</i> , 2008, 154, 1158-1165.	6.5	20
3029	Synthesis, characterization, DNA-binding and spectral properties of complexes [Ru(L)4(dppz)]2+ (L=Im) Tj ETQq0 0,0,rgBT /Overlock 10	1.5	118
3030	QM/MM investigation of structure and spectroscopic properties of a vanadium-containing peroxidase. <i>Journal of Inorganic Biochemistry</i> , 2008, 102, 1684-1690.	1.5	32
3031	Both Met(109) and Met(112) are utilized for Cu(II) coordination by the amyloidogenic fragment of the human prion protein at physiological pH. <i>Journal of Inorganic Biochemistry</i> , 2008, 102, 2103-2113.	1.5	29
3032	Theoretical exploration of the photosensitive properties of xanthurenic acid, a tryptophan metabolite in cataractous human lenses. <i>Dyes and Pigments</i> , 2008, 76, 646-649.	2.0	13
3033	QSAR, action mechanism and molecular design of flavone and isoflavone derivatives with cytotoxicity against HeLa. <i>European Journal of Medicinal Chemistry</i> , 2008, 43, 2159-2170.	2.6	22
3034	Photodetachment and Lysine vis spectral properties of chromophore containing = st1.gif" display="inline" overflow=" scroll" xmlns:xocs= "http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tbl="http://www.elsevier.com/xml/common/table/dtd" xmlns:tbl_struct="http://www.elsevier.com/xml/common/table-struct/dtd" style="float: right; font-size: small;">	1.2	17
3035	Theoretical study on the reaction of bromine-substituted ethanes with hydrogen atoms. <i>Chemical Physics Letters</i> , 2008, 455, 20-25.	1.2	1
3036	Analytical representation of the Becke-Roussel exchange functional. <i>Chemical Physics Letters</i> , 2008, 455, 103-109.	1.2	25

#	ARTICLE	IF	CITATIONS
3037	Mechanism for the gas-phase reaction between NO ₃ and furan: A theoretical study. <i>Chemical Physics Letters</i> , 2008, 455, 164-168.	1.2	7
3038	Theoretical studies on the structure and effective exchange integral (J_{ab}) of an active site in oxyhemocyanin (oxyHc) by using approximately spin-projected geometry optimization (AP-opt) method. <i>Chemical Physics Letters</i> , 2008, 456, 76-79.	1.2	14
3039	Computational study on the kinetics of the reaction between Ca ²⁺ and urea. <i>Chemical Physics Letters</i> , 2008, 456, 156-161.	1.2	14
3040	DFT study on the gas phase reaction of Ni ⁺ with CS ₂ . <i>Chemical Physics Letters</i> , 2008, 458, 19-23.	1.2	10
3041	How does the Fe ⁺ -mediated demethanation of CH ₃ OCH ₃ occurs? A density functional theoretical study. <i>Chemical Physics Letters</i> , 2008, 459, 33-38.	1.2	12
3042	The protovalent NO bond: Quantum chemical topology (QCT of ELF and ELI-D) study on the bonding in the nitrous acid HONO and its relevancy to the experiment. <i>Chemical Physics Letters</i> , 2008, 460, 559-562.	1.2	14
3043	C ⁺ activation of C ₂ H ₄ by V^+ in the gas phase: A case of two-state reactivity process. <i>Chemical Physics Letters</i> , 2008, 463, 309-314.	1.2	7
3044	A theoretical study on the gas phase reaction of Au ⁺ with CH ₃ F. <i>Chemical Physics Letters</i> , 2008, 463, 334-339.	1.2	23
3045	Sr ²⁺ -neutral molecules interactions: An assessment of theoretical procedures. <i>Chemical Physics Letters</i> , 2008, 464, 240-244.	1.2	10
3046	Magnetic interactions in dehydrogenated Guanine-Cytosine base pair. <i>Chemical Physics Letters</i> , 2008, 465, 285-289.	1.2	10
3047	Computational studies on the mechanisms for the gas-phase reaction between thiophene and NO ₃ . <i>Chemical Physics Letters</i> , 2008, 467, 52-57.	1.2	7
3048	Synthesis, dopaminergic profile, and molecular dynamics calculations of N-alkyl substituted 2-aminoindans. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 3233-3244.	1.4	10
3049	A comparative study of single reference correlation methods of the coupled-pair type. <i>Chemical Physics</i> , 2008, 343, 217-230.	0.9	96
3050	Theoretical energetic and vibrational analysis of amide-templated pseudorotaxanes. <i>Chemical Physics</i> , 2008, 343, 186-199.	0.9	9
3051	Pigment Yellow 101: A showcase for photo-initiated processes in medium-sized molecules. <i>Chemical Physics</i> , 2008, 347, 472-482.	0.9	36
3052	Hydrogen and dihydrogen bonding of transition metal hydrides. <i>Chemical Physics</i> , 2008, 345, 95-102.	0.9	30
3053	51V solid-state NMR investigations and DFT studies of model compounds for vanadium haloperoxidases. <i>Solid State Nuclear Magnetic Resonance</i> , 2008, 34, 52-67.	1.5	29
3054	Molecular level investigation of 2,2,6,6-tetramethyl-3,5-heptanedione on Si(100)-2 \times 1: Spectroscopic and computational studies. <i>Surface Science</i> , 2008, 602, 2222-2231.	0.8	5

#	ARTICLE	IF	CITATIONS
3055	First-principles calculations-based model for the reactive ion etching of metal oxide surfaces. <i>Vacuum</i> , 2008, 83, 599-601.	1.6	9
3056	Total synthesis of the antimalarial naphthylisoquinoline alkaloid 5-epi-4- ϵ^2 -O-demethylancistrobertsonine C by asymmetric Suzuki cross-coupling. <i>Tetrahedron</i> , 2008, 64, 5563-5568.	1.0	45
3057	Sigmatropic shifts and cycloadditions on neutral, cationic, and anionic pentadienyl+butadiene potential energy surfaces. <i>Tetrahedron</i> , 2008, 64, 5672-5679.	1.0	16
3058	Synthesis of cyclopropane-annulated conduritol derivatives: norcaran-2,3,4,5-tetraoles. <i>Tetrahedron</i> , 2008, 64, 7289-7294.	1.0	15
3059	New chiral tetraaza ligands for the efficient enantioselective addition of dialkylzinc to aromatic aldehydes. <i>Tetrahedron</i> , 2008, 64, 9717-9724.	1.0	34
3060	Theoretical studies of stereoselectivities in the direct anti- and syn-aldol reactions catalyzed by different amino acid derivatives. <i>Tetrahedron: Asymmetry</i> , 2008, 19, 1288-1296.	1.8	20
3061	Theoretical studies of stereoselectivities in the direct syn- and anti-Mannich reactions catalyzed by different amino acids. <i>Tetrahedron: Asymmetry</i> , 2008, 19, 2285-2292.	1.8	15
3062	Conformational study of the 1,2,3-propanetriol (glycerol) in the channel of the aquaglyceroporin GlpF. <i>Computational and Theoretical Chemistry</i> , 2008, 850, 21-31.	1.5	1
3063	Molecular structure and vibrational spectra of indole and 5-aminoindole by density functional theory and ab initio Hartree-Fock calculations. <i>Computational and Theoretical Chemistry</i> , 2008, 850, 84-93.	1.5	45
3064	Theoretical study on the reaction of Mn ⁺ (7S and 5S states) with COS. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 127-133.	1.5	5
3065	Photophysical and photochemical properties of anthraquinones: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 220-224.	1.5	12
3066	Computational study on the mechanism for the reaction of OH with 2-methylfuran. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 353-357.	1.5	22
3067	Silicon-sodium binary clusters SinNa (n=1/2, 10) and their anions: Structures, thermochemistry, and electron affinities. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 197-206.	1.5	17
3068	Ab initio study of hydrogen abstraction reactions on toluene and tetralin. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 232-241.	1.5	8
3069	Geometries and electronic properties of clusters. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 348-352.	1.5	6
3070	Theoretical exploration on quenching mechanisms of triplet state riboflavin by xanthone derivatives. <i>Computational and Theoretical Chemistry</i> , 2008, 854, 106-109.	1.5	2
3071	The selenium clusters Sen (n=1-5) and their anions: Structures and electron affinities. <i>Computational and Theoretical Chemistry</i> , 2008, 854, 89-105.	1.5	17
3072	A thermodynamic investigation of DPPH radical-scavenging mechanisms of folates. <i>Computational and Theoretical Chemistry</i> , 2008, 856, 119-123.	1.5	23

#	ARTICLE	IF	CITATIONS
3073	Theoretical study of activation Fe-O bond of FeO+ by CO in the gas phase. Computational and Theoretical Chemistry, 2008, 858, 26-30.	1.5	4
3074	Monocation-driven proton transfer relays within G protein-coupled receptors of the rhodopsin class and the GTP synthase mechanism. Computational and Theoretical Chemistry, 2008, 859, 51-68.	1.5	2
3075	The effects of oxidation and protonation on the N-glycosidic bond stability of 8-oxo-2-deoxyguanosine: DFT study. Computational and Theoretical Chemistry, 2008, 860, 52-57.	1.5	13
3076	A theoretical study on the gas phase reaction of La+ with CS2. Computational and Theoretical Chemistry, 2008, 861, 142-146.	1.5	2
3077	Theoretical investigation on the triplet excited state properties of the porphyrin-related photosensitizers and the implications in illustrating their photosensitization mechanisms. Computational and Theoretical Chemistry, 2008, 862, 130-132.	1.5	10
3078	Structures, electron affinities, and vibrational frequencies of the mono-, di-substituted SF6 radicals. Computational and Theoretical Chemistry, 2008, 863, 28-32.	1.5	5
3079	A TDDFT and PCM-TDDFT studies on absorption spectra of N-substituted 1,8-naphthalimides dyes. Computational and Theoretical Chemistry, 2008, 865, 79-87.	1.5	22
3080	Quantum chemical studies on the inhibition of corrosion of copper surface by substituted uracils. Applied Surface Science, 2008, 255, 2433-2441.	3.1	206
3081	Time-dependent density functional study of excimers and exciplexes of organic molecules. Chemical Physics, 2008, 343, 362-371.	0.9	78
3082	Fluorescein isothiocyanate: Molecular characterization by theoretical calculations. Chemical Physics, 2008, 354, 155-161.	0.9	17
3083	Reaction of carbon monoxide with tri-tert-butylgallium: The first example of CO insertion into a gallium-carbon bond. Inorganica Chimica Acta, 2008, 361, 3332-3337.	1.2	16
3084	Some considerations on the proper use of computational tools in transition metal chemistry. Inorganica Chimica Acta, 2008, 361, 3820-3831.	1.2	71
3085	Selecting fixed-charge groups for electron-based peptide dissociations. International Journal of Mass Spectrometry, 2008, 276, 127-135.	0.7	14
3086	Electron capture, femtosecond electron transfer and theory: A study of noncovalent crown ether 1,n-diammonium alkane complexes. International Journal of Mass Spectrometry, 2008, 276, 116-126.	0.7	32
3087	Azoxybenzene rearrangement catalyzed by solid acids. Journal of Molecular Catalysis A, 2008, 292, 36-43.	4.8	3
3088	Synthesis, characterization, structural optimization using density functional theory and superoxide ion scavenging activity of some Schiff bases. Journal of Molecular Structure, 2008, 873, 5-16.	1.8	48
3089	Experimental and theoretical studies on the DNA-binding and spectral properties of water-soluble complex [Ru(Melm)4(dpq)]2+. Journal of Molecular Structure, 2008, 881, 156-166.	1.8	68
3090	An unusual binding mode of a guanidinate ligand in a species with a short metal-metal single bond. Journal of Molecular Structure, 2008, 890, 3-8.	1.8	9

#	ARTICLE	IF	CITATIONS
3091	Synthesis and conformational analysis of phenyl-substituted 1,3,2-oxazaphosphino[4,3-a]- and 1,2,3-oxathiazino[4,3-a]isoquinolines. <i>Journal of Molecular Structure</i> , 2008, 888, 124-137.	1.8	2
3092	Vibrational calculations for the H ₂ O ⋯ CO complex. <i>Journal of Molecular Structure</i> , 2008, 887, 172-179.	1.8	18
3093	Orbital-dependent density functionals: Theory and applications. <i>Reviews of Modern Physics</i> , 2008, 80, 3-60.	16.4	1,069
3094	Photoelectrochemical Properties of Doubly \hat{I}^2 -Functionalized Porphyrin Sensitizers for Dye-Sensitized Nanocrystalline-TiO ₂ Solar Cells. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16691-16699.	1.5	126
3095	Excited states of thiophene: ring opening as deactivation mechanism. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 380-392.	1.3	86
3096	Magnetic and Optical Properties of Cu(II) \hat{B} is(oxamato) Complexes: Combined Quantum Chemical Density Functional Theory and Vibrational Spectroscopy Studies. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5585-5593.	1.2	10
3097	Very Large Difference in Electronic Communication of Dimetal Species with Heterobiphenylene and Heteroanthracene Units. <i>Inorganic Chemistry</i> , 2008, 47, 219-229.	1.9	22
3098	Mechanistic possibilities for oxetane formation in the biosynthesis of Taxol TM 's D ring. <i>Russian Journal of General Chemistry</i> , 2008, 78, 723-731.	0.3	15
3099	Quantum-chemical calculation of steric structure of the complexes formed at template synthesis in three-component systems of Co(II) [Ni(II), Cu(II)] ion-bithiooxamide-acetone. <i>Russian Journal of General Chemistry</i> , 2008, 78, 1849-1861.	0.3	12
3100	Adsorption properties of oxidized gallium-modified zeolite ZSM-5 from diffuse-reflectance IR-spectroscopic and quantum-chemical data: II. Interaction with carbon monoxide and water. <i>Kinetics and Catalysis</i> , 2008, 49, 149-155.	0.3	3
3101	Hydrolysis of nerve agents by model nucleophiles: A computational study. <i>Chemico-Biological Interactions</i> , 2008, 175, 200-203.	1.7	18
3102	Absorption Spectrum of OH Radical in Water. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13372-13381.	1.1	38
3103	Anionic Oligomerization of Ethylene over Ga/ZSM-5 Zeolite: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 19604-19611.	1.5	26
3104	E ₂ and S _N 2 Reactions of X ⁺ + CH ₃ CH ₂ X (X = F, Cl); an <i>ab Initio</i> and DFT Benchmark Study. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 929-940.	2.3	86
3105	The role of cap chirality in the mechanism of growth of single-wall carbon nanotubes. <i>Nanotechnology</i> , 2008, 19, 485604.	1.3	37
3106	DFT Approach to the Calculation of Mössbauer Isomer Shifts. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 278-285.	2.3	40
3107	Toward Understanding the Nature of Internal Rotation Barriers with a New Energy Partition Scheme: Ethane and <i>n</i> -Butane. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6690-6699.	1.1	90
3108	Variation of Average <i>g</i> Values and Effective Exchange Coupling Constants among [2Fe ²⁺ S] Clusters: A Density Functional Theory Study of the Impact of Localization (Trapping Forces) versus Delocalization (Double-Exchange) as Competing Factors. <i>Inorganic Chemistry</i> , 2008, 47, 5394-5416.	1.9	43

#	ARTICLE	IF	CITATIONS
3109	Periodic DFT and High-Resolution Magic-Angle-Spinning (HR-MAS) ¹ H NMR Investigation of the Active Surfaces of MgCl ₂ -Supported Ziegler-Natta Catalysts. The MgCl ₂ Matrix. <i>Journal of Physical Chemistry C</i> , 2008, 112, 1081-1089.	1.5	123
3110	A ¹² -Naphthaleneimide-Modified Terthiophene Exhibiting Charge Transfer and Polarization Through the Short Molecular Axis. Joint Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6732-6740.	1.1	27
3111	Hydrogen-Bonding Interactions in 2-Thiophen-3-ylmalonic Acid. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10650-10656.	1.1	7
3112	Ab Initio and Coupled-Perturbed Density Functional Theory Estimation of Zero-Field Splittings in MnII Transition Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7976-7983.	1.1	76
3113	Detailed Assignment of the Magnetic Circular Dichroism and UV-vis Spectra of Five-Coordinate High-Spin Ferric [Fe(TPP)(Cl)]. <i>Inorganic Chemistry</i> , 2008, 47, 4963-4976.	1.9	72
3114	The AM05 density functional applied to solids. <i>Journal of Chemical Physics</i> , 2008, 128, 084714.	1.2	220
3115	Hybrid exchange-correlation functional for accurate prediction of the electronic and structural properties of ferroelectric oxides. <i>Physical Review B</i> , 2008, 77, .	1.1	315
3116	Aromatic C-H Activation and Catalytic Hydrophenylation of Ethylene by TpRu{P(OCH ₂) ₃ CEt}(NCMe)Ph. <i>Organometallics</i> , 2008, 27, 3007-3017.	1.1	55
3117	Size-dependence of Fermi energy of gold nanoparticles loaded on titanium(IV) dioxide at photostationary state. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 6553.	1.3	78
3118	Nature and magnitude of aromatic stacking of nucleic acid bases. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2595.	1.3	317
3119	Atomic and Electronic Structure of Cerium Oxide Stepped Model Surfaces. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17643-17651.	1.5	40
3120	The densities produced by the density functional theory: Comparison to full configuration interaction. <i>Journal of Chemical Physics</i> , 2008, 128, 034102.	1.2	30
3121	The importance of the oxidative character of doubly charged metal cations in binding neutral bases. [Urea-M] ₂ ⁺ and [thiourea-M] ₂ ⁺ (M = Mg, Ca, Cu) complexes. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 3229.	1.3	39
3122	The Role of Dangling Bonds in H ₂ O-Induced Oxidation of Si(100)-2 × 1. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9434-9442.	1.5	17
3123	Crystal structure prediction could have helped the experimentalists with polymorphism in benzamide. <i>Molecular Simulation</i> , 2008, 34, 1359-1370.	0.9	18
3124	Generalized gradient approximation model exchange holes for range-separated hybrids. <i>Journal of Chemical Physics</i> , 2008, 128, 194105.	1.2	238
3125	Density Functional Theory in Transition-Metal Chemistry: Relative Energies of Low-Lying States of Iron Compounds and the Effect of Spatial Symmetry Breaking. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 307-315.	2.3	86
3126	Adsorption and Interfacial Chemistry of Pentacene on the Clean Si(100) Surface: A Density Functional Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6033-6048.	1.5	11

#	ARTICLE	IF	CITATIONS
3127	Exploring the origin of the internal rotational barrier for molecules with one rotatable dihedral angle. <i>Journal of Chemical Physics</i> , 2008, 129, 094104.	1.2	59
3128	Prediction of metastable metal-rare gas fluorides: FMRgF (M=Be and Mg; Rg=Ar, Kr and Xe). <i>Journal of Chemical Physics</i> , 2008, 128, 144314.	1.2	32
3129	DFT Calculations of ⁵¹ V Solid-State NMR Parameters of Vanadium(V) Model Complexes. <i>Zeitschrift Fur Physikalische Chemie</i> , 2008, 222, 1389-1406.	1.4	18
3130	Electronic Nature of Carbonium Ions and Their Silicon Analogues. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3165-3171.	1.1	10
3131	Studies on adsorption of mono- and multi-chromophoric hemicyanine dyes on silver nanoparticles by surface-enhanced resonance raman and theoretical calculations. <i>Journal of Chemical Physics</i> , 2008, 129, 184702.	1.2	25
3132	Assessment of Density Functionals for Intramolecular Dispersion-Rich Interactions. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1610-1619.	2.3	65
3133	Ab initio studies of structural and electronic properties. , 2008, , 17-54.		2
3134	Performance of the Density Functional Theory/Multireference Configuration Interaction Method on Electronic Excitation of Extended π -Systems. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1501-1515.	2.3	164
3135	The Coupling of Isonitriles and Carboxylic Acids Occurring By Sequential Concerted Rearrangement Mechanisms. <i>Organic Letters</i> , 2008, 10, 4093-4096.	2.4	62
3136	Exchange of Organic Radicals with Organo-Cobalt Complexes Formed in the Living Radical Polymerization of Vinyl Acetate. <i>Journal of the American Chemical Society</i> , 2008, 130, 13373-13381.	6.6	96
3137	NMR chemical shifts of molecules encapsulated in single walled carbon nanotubes. <i>Journal of Chemical Physics</i> , 2008, 128, 101102.	1.2	33
3138	Tuning the Activity of Zn(II) Complexes in DNA Cleavage: Clues for Design of New Efficient Metallo-Hydrolases. <i>Inorganic Chemistry</i> , 2008, 47, 5473-5484.	1.9	52
3139	Combined Ligand Field and Density Functional Theory Analysis of the Magnetic Anisotropy in Oligonuclear Complexes Based on Fe ^{III} -CN ⁻ M ^{II} Exchange-Coupled Pairs. <i>Inorganic Chemistry</i> , 2008, 47, 2449-2463.	1.9	78
3140	[12]Annulene Radical Anions Revisited: Evaluation of Structure Assignments Based on Computed Energetic and Electron Spin Resonance Data. <i>Journal of Organic Chemistry</i> , 2008, 73, 8745-8754.	1.7	0
3141	A Dramatic Switch of Enantioselectivity in Asymmetric Heck Reaction by Benzylic Substituents of Ligands. <i>Journal of the American Chemical Society</i> , 2008, 130, 9717-9725.	6.6	116
3142	Chiral Aromaticities. A Topological Exploration of Möbius Homoaromaticity. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1841-1848.	2.3	23
3143	The Degradation Pathways in Chloride Medium of the Third Generation Anticancer Drug Oxaliplatin. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10765-10768.	1.2	40
3144	A Structural and Theoretical Study of the Thiophosphinite and Dithiophosphinate Anions. Phosphorus, Sulfur and Silicon and the Related Elements, 2008, 183, 2685-2702.	0.8	3

#	ARTICLE	IF	CITATIONS
3145	Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrroline <i>N</i> -Oxide. 4. Conformational Effects on the EPR Hyperfine Splitting Constants. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12607-12615.	1.1	26
3146	An ab initio and Density Functional Theory Study of Radical-Clock Reactions. <i>Journal of Organic Chemistry</i> , 2008, 73, 1536-1545.	1.7	13
3147	Competing C–F Activation Pathways in the Reaction of Pt(0) with Fluoropyridines: Phosphine-Assistance versus Oxidative Addition. <i>Journal of the American Chemical Society</i> , 2008, 130, 15499-15511.	6.6	101
3148	Recent developments in proton exchange membranes for fuel cells. <i>Energy and Environmental Science</i> , 2008, 1, 101.	15.6	462
3149	Origin of Enantioselection in Hetero-Diels–Alder Reactions Catalyzed by Naphthyl-TADDOL. <i>Organic Letters</i> , 2008, 10, 2749-2752.	2.4	78
3150	Nitrogen Monoxide Interaction with Cu(I) Sites in Zeolites X and Y: Quantum Chemical Calculations and IR Studies. <i>Journal of Physical Chemistry C</i> , 2008, 112, 17998-18010.	1.5	30
3151	Selenourea–Ca ²⁺ Reactions in Gas Phase. Similarities and Dissimilarities with Urea and Thiourea. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5479-5486.	1.2	26
3152	Using a Two-Step Hydride Transfer To Achieve 1,4-Reduction in the Catalytic Hydrogenation of an Acyl Pyridinium Cation. <i>Journal of Organic Chemistry</i> , 2008, 73, 9668-9674.	1.7	34
3153	On the Bonding of Selenocyanates and Isoselenocyanates and Their Protonated Derivatives. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1593-1599.	2.3	8
3154	Laser-induced nuclear magnetic resonance splitting in hydrocarbons. <i>Journal of Chemical Physics</i> , 2008, 129, 124102.	1.2	26
3155	Thioflavin T Hydroxylation at Basic pH and Its Effect on Amyloid Fibril Detection. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15174-15181.	1.2	100
3156	Electronic Structure Characteristics of ESIPT and TICT Fluorescence Emissions and Calculations of Emitting Energies. <i>Acta Physico-chimica Sinica</i> , 2008, 24, 552-560.	0.6	11
3157	Computational Studies on Biosynthetic Carbocation Rearrangements Leading to Sativene, Cyclosativene, Î±-Ylangene, and Î²-Ylangene. <i>Journal of Organic Chemistry</i> , 2008, 73, 6570-6579.	1.7	57
3158	Rydberg energies using excited state density functional theory. <i>Journal of Chemical Physics</i> , 2008, 129, 124112.	1.2	49
3159	Sulfoxide, Sulfur, and Nitrogen Oxidation and Dealkylation by Cytochrome P450. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1369-1377.	2.3	83
3160	Approximation to density functional theory for the calculation of band gaps of semiconductors. <i>Physical Review B</i> , 2008, 78, .	1.1	381
3161	Application of 1-Aminocyclohexane Carboxylic Acid to Protein Nanostructure Computer Design. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 333-343.	2.5	19
3162	Electronically excited states of water clusters of 7-azaindole: Structures, relative energies, and electronic nature of the excited states. <i>Journal of Chemical Physics</i> , 2008, 128, 214310.	1.2	18

#	ARTICLE	IF	CITATIONS
3163	Nature of the Fe ²⁺ Bonding in Oxy-Myoglobin: Effect of the Protein. <i>Journal of the American Chemical Society</i> , 2008, 130, 14778-14790.	6.6	234
3164	Quantum Mechanical/Molecular Mechanical Study of Mechanisms of Heme Degradation by the Enzyme Heme Oxygenase: The Strategic Function of the Water Cluster. <i>Journal of the American Chemical Society</i> , 2008, 130, 1953-1965.	6.6	71
3165	Compound I in Heme Thiolate Enzymes: A Comparative QM/MM Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13128-13138.	1.1	32
3166	Gating of single molecule transistors: Combining field-effect and chemical control. <i>Journal of Chemical Physics</i> , 2008, 128, 154706.	1.2	26
3167	Hydrogen Bonding Lowers Intrinsic Nucleophilicity of Solvated Nucleophiles. <i>Journal of the American Chemical Society</i> , 2008, 130, 15038-15046.	6.6	60
3168	Core-excitation energy calculations with a long-range corrected hybrid exchange-correlation functional including a short-range Gaussian attenuation (LCgau-BOP). <i>Journal of Chemical Physics</i> , 2008, 129, 184113.	1.2	73
3170	Local molecular orbitals and hyper-susceptibility of TeO ₂ glass. <i>Journal of Non-Crystalline Solids</i> , 2008, 354, 199-202.	1.5	26
3171	Synthesis and density functional theoretical study of steroidal spiro-triazolidinone. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2008, 110, 278-283.	1.2	6
3172	Local correlation functional for electrons in two dimensions. <i>Physical Review B</i> , 2008, 78, .	1.1	25
3173	Chapter 17 The Supporting Role of Molecular Modelling and Computational Chemistry in Polymer Analysis. <i>Comprehensive Analytical Chemistry</i> , 2008, 53, 685-734.	0.7	0
3174	Triplet Pathways in Diarylethene Photochromism: Photophysical and Computational Study of Dyads Containing Ruthenium(II) Polypyridine and 1,2-Bis(2-methylbenzothiophene-3-yl)maleimide Units. <i>Journal of the American Chemical Society</i> , 2008, 130, 7286-7299.	6.6	163
3175	A Measure for σ -Donor and π -Acceptor Properties of Diiminepyridine-Type Ligands. <i>Organometallics</i> , 2008, 27, 2699-2705.	1.1	36
3176	Fine Synthetic Nucleoside Chemistry Based on Nucleoside Natural Products Synthesis. <i>Chemical and Pharmaceutical Bulletin</i> , 2008, 56, 1059-1072.	0.6	28
3177	Effect of Metal Ions (Li ⁺ , Na ⁺ , K ⁺ , Mg ²⁺), Tj ETQq1 1 0.784314 rgBT /Overlock 1 on the Structure and Properties of α -Arginine and Zwitterionic α -Arginine. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7652-7661.	1.1	41
3178	Reactions of the hydroperoxide anion with dimethyl methylphosphonate in an ion trap mass spectrometer: evidence for a gas phase β -effect. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 2316.	1.5	49
3179	Interaction of Ca ²⁺ with uracil and its thio derivatives in the gas phase. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 3695.	1.5	40
3180	Organocatalytic Asymmetric Synthesis of β , γ -Disubstituted β -Amino Acids and Derivatives. <i>Journal of the American Chemical Society</i> , 2008, 130, 12031-12037.	6.6	173
3181	QM/MM \hat{P} BSA Method To Estimate Free Energies for Reactions in Proteins. <i>Journal of Physical Chemistry B</i> , 2008, 112, 12537-12548.	1.2	55

#	ARTICLE	IF	CITATIONS
3182	1,3-Dipolar Cycloaddition of Organic Azides to Alkynes by a Dicopper-Substituted Silicotungstate. <i>Journal of the American Chemical Society</i> , 2008, 130, 15304-15310.	6.6	155
3183	Cu ²⁺ Cation Coordination to Adenine-Thymine Base Pair. Effects on Intermolecular Proton-Transfer Processes. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4817-4825.	1.2	52
3184	Amine-Functionalized Task-Specific Ionic Liquids: A Mechanistic Explanation for the Dramatic Increase in Viscosity upon Complexation with CO ₂ from Molecular Simulation. <i>Journal of the American Chemical Society</i> , 2008, 130, 14690-14704.	6.6	382
3185	Assessment of correction methods for the band-gap problem and for finite-size effects in supercell defect calculations: Case studies for ZnO and GaAs. <i>Physical Review B</i> , 2008, 78, .	1.1	1,035
3186	Quantum chemical studies on the potentially important imidates. <i>Computational and Theoretical Chemistry</i> , 2008, 861, 62-67.	1.5	1
3187	Environmental Photochemistry of Nitro-PAHs: Direct Observation of Ultrafast Intersystem Crossing in 1-Nitropyrene. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6313-6319.	1.1	89
3188	Thermal C ² →C ⁶ Cyclization of Enyne Carbodiimides: Experimental Evidence Contradicts a Diradical and Suggests a Carbene Intermediate. <i>Journal of Organic Chemistry</i> , 2008, 73, 3005-3016.	1.7	35
3189	Construction of a generalized gradient approximation by restoring the density-gradient expansion and enforcing a tight Lieb-Oxford bound. <i>Journal of Chemical Physics</i> , 2008, 128, 184109.	1.2	260
3190	Influence of Sequential Guanidinium Methylation on the Energetics of the Guanidinium-Guanine Dimer and Guanidinium-Guanine-Cytosine Trimer: Implications for the Control of Protein-DNA Interactions by Arginine Methyltransferases. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16995-17002.	1.2	3
3191	Conformational Preferences of \pm -Substituted Proline Analogues. <i>Journal of Organic Chemistry</i> , 2008, 73, 3418-3427.	1.7	42
3192	Theoretical study of one-photon and two-photon absorption properties of perylene tetracarboxylic derivatives. <i>Journal of Chemical Physics</i> , 2008, 129, 014301.	1.2	23
3193	A Conclusive Mechanism of the Photoinduced Reaction Cascade in Blue Light Using Flavin Photoreceptors. <i>Journal of the American Chemical Society</i> , 2008, 130, 12501-12513.	6.6	103
3194	Insights into DNA Binding of Ruthenium Arene Complexes: Role of Hydrogen Bonding and π -Stacking. <i>Inorganic Chemistry</i> , 2008, 47, 3893-3902.	1.9	36
3195	Design and Synthesis of Propeller-Shaped Dispiroisoxazolinopiperidinochromanones. <i>ACS Combinatorial Science</i> , 2008, 10, 225-229.	3.3	15
3196	Novofumigatonin, a New Orthoester Meroterpenoid from <i>Aspergillus novofumigatus</i> . <i>Organic Letters</i> , 2008, 10, 401-404.	2.4	38
3197	Theoretical Study on the Conformational Conversion of 1,3-Dioxane Inside a Capsular Host. <i>Chemical Research in Chinese Universities</i> , 2008, 24, 241-245.	1.3	1
3198	Dynamics and magnetic resonance properties of Sc ₃ C ₂ @C ₈₀ and its monoanion. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 7158.	1.3	31
3199	A dramatic difference between the electron-driven dissociation of alcohols and ethers and its relation to Rydberg states. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5232.	1.3	25

#	ARTICLE	IF	CITATIONS
3200	The non-covalent functionalisation of carbon nanotubes studied by density functional and semi-empirical molecular orbital methods including dispersion corrections. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 128-135.	1.3	30
3201	A QM/MM study of fluoroaromatic interactions at the binding site of carbonic anhydrase II, using a DFT method corrected for dispersive interactions. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2706.	1.3	20
3202	A DFT study of EPR parameters in Cu(II) complexes of the octarepeat region of the prion protein. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 4573.	1.3	26
3203	Structure-Property Investigations of Conjugated Thiophenes Fused onto a Dehydro[14]annulene Scaffold. <i>Journal of Organic Chemistry</i> , 2008, 73, 4424-4432.	1.7	22
3204	Is the FeO ₂ ²⁻ Anion Bent or Linear?. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13641-13649.	1.1	22
3205	Microhydration of X ₂ Gas (X = Cl, Br, and I): A Theoretical Study on X ₂ ·nH ₂ O Clusters (n = 1-8). <i>Journal of Physical Chemistry A</i> , 2008, 112, 744-751.	1.1	29
3206	Structures, Electron Affinities, and Harmonic Vibrational Frequencies of the Simplest Alkyl Peroxyl Radicals and Their Anions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6999-7014.	1.1	6
3207	Anodic oxidation of indenofluorene. Electrodeposition of electroactive poly(indenofluorene). <i>New Journal of Chemistry</i> , 2008, 32, 1259.	1.4	20
3208	Protonation of the Proximal Histidine Ligand in Heme Peroxidases. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2501-2510.	1.2	29
3209	Potent <i>cis</i> -Locked Bithiazole Correctors of F508 Cystic Fibrosis Transmembrane Conductance Regulator Cellular Processing for Cystic Fibrosis Therapy. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 6044-6054.	2.9	49
3210	Combined Experimental and Theoretical Study of the Mechanism and Enantioselectivity of Palladium-Catalyzed Intermolecular Heck Coupling. <i>Journal of the American Chemical Society</i> , 2008, 130, 10414-10421.	6.6	97
3211	Kinetics of the Initial Oxidation of the (0001) 6H-SiC (3 × 3) Reconstructed Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16864-16868.	1.5	5
3212	Solvation of Propylene Oxide in Water: Vibrational Circular Dichroism, Optical Rotation, and Computer Simulation Studies. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5621-5627.	1.1	87
3213	Intrinsic Conformational Preferences of <i>trans</i> -Dibenzylglycine. <i>Journal of Organic Chemistry</i> , 2008, 73, 4205-4211.	1.7	10
3214	Effect of Nanotube Length on the Aromaticity of Single-Wall Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3482-3488.	1.5	19
3215	An Investigation of the Accuracy of Different DFT Functionals on the Water Exchange Reaction in Hydrated Uranyl(VI) in the Ground State and the First Excited State. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 569-577.	2.3	64
3216	DFT Investigation on the Mechanism of the Deacetylation Reaction Catalyzed by LpxC. <i>Journal of Physical Chemistry B</i> , 2008, 112, 3462-3469.	1.2	26
3217	Range Separation and Local Hybridization in Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12530-12542.	1.1	94

#	ARTICLE	IF	CITATIONS
3218	Free Radical Formation in Supercritical CO ₂ , Using Muonium as a Probe and Implication for H Atom Reaction with Ethene. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4593-4600.	1.1	12
3219	Understanding the Planar Tetracoordinate Carbon Atom: A Spiropentadiene Dication. <i>Journal of Physical Chemistry A</i> , 2008, 112, 686-692.	1.1	17
3220	Competing Gas-Phase Substitution and Elimination Reactions of Gemini Surfactants with Anionic Counterions by Mass Spectrometry. Density Functional Theory Correlations with Their Bolaform Halide Salt Models. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14435-14445.	1.2	13
3221	Interaction of Molecular Hydrogen with Open Transition Metal Centers for Enhanced Binding in Metal-Organic Frameworks: A Computational Study. <i>Inorganic Chemistry</i> , 2008, 47, 4032-4044.	1.9	48
3222	Conductance of a Cobalt(II) Terpyridine Complex Based Molecular Transistor: A Computational Analysis. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2043-2048.	1.1	22
3223	A Density Functional Theory Investigation on the Mechanism of the Second Half-Reaction of Nitric Oxide Synthase. <i>Journal of the American Chemical Society</i> , 2008, 130, 3328-3334.	6.6	30
3224	Quantum Mechanical/Molecular Mechanical Study on the Mechanisms of Compound I Formation in the Catalytic Cycle of Chloroperoxidase: An Overview on Heme Enzymes. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9490-9500.	1.2	60
3225	Structure of Diethyl Phosphate Bound to the Binuclear Metal Center of Phosphotriesterase. <i>Biochemistry</i> , 2008, 47, 9497-9504.	1.2	67
3226	1-Amino-2-Phenylcyclopentane-1-carboxylic Acid: A Conformationally Restricted Phenylalanine Analogue. <i>Journal of Organic Chemistry</i> , 2008, 73, 644-651.	1.7	11
3227	Experimental and Theoretical Studies on the Complexes of [Pb(<i>m</i> -Pyridyl)] ⁺ (<i>m</i> = 1-4). <i>Journal of Physical Chemistry A</i> , 2008, 112, 6850-6858.	1.1	5
3228	Variability of Chain Transfer to Monomer Step in Olefin Polymerization. <i>Organometallics</i> , 2008, 27, 4098-4107.	1.1	59
3229	On the Importance of Electron Correlation Effects for the Intramolecular Stacking Geometry of a Bis-Thiophene Derivative. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12469-12474.	1.1	23
3230	Computational Study of the Small Zr(IV) Polynuclear Species. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 145-155.	2.3	10
3231	On the Electronic Structure and Chemical Bonding in the Tantalum Trimer Cluster. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10962-10967.	1.1	47
3232	Mechanism on Two-Electron Oxidation of Ubiquinol at the Q _p Site in Cytochrome <i>bc</i> ₁ Complex: B3LYP Study with Broken Symmetry. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15116-15126.	1.2	15
3233	Driving Force for the Adsorption of Sexithiophene on Gold. <i>Journal of Physical Chemistry C</i> , 2008, 112, 19516-19520.	1.5	11
3234	Gas-Phase Reactions of Co ⁺ with Ethylamine: A Theoretical Approach to the Reaction Mechanisms of Transition Metal Ions with Primary Amines. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5312-5321.	1.1	15
3235	Theoretical Investigation of the Electronic Asymmetry of the Special Pair Cation Radical in the Photosynthetic Type-II Reaction Center. <i>Journal of Physical Chemistry B</i> , 2008, 112, 13923-13933.	1.2	25

#	ARTICLE	IF	CITATIONS
3236	Peptide Hydrolysis by the Binuclear Zinc Enzyme Aminopeptidase from <i>Aeromonas proteolytica</i> : A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2494-2500.	1.2	68
3237	Computational Study of Iron Bis(dithiolene) Complexes: Redox Non-Innocent Ligands and Antiferromagnetic Coupling. <i>Inorganic Chemistry</i> , 2008, 47, 10037-10045.	1.9	16
3238	Spectroscopic and Computational Investigation of Second-Sphere Contributions to Redox Tuning in <i>Escherichia coli</i> Iron Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2008, 47, 3978-3992.	1.9	33
3239	Stacking and Solvent Effects on the Electronic and Optical Properties of Gold and Mercury Acetylide Aggregations: A Theoretical Study. <i>Organometallics</i> , 2008, 27, 4636-4648.	1.1	16
3240	Excitation Energies from Spin-Restricted Ensemble-Referenced Kohn-Sham Method: A State-Average Approach. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12980-12988.	1.1	55
3241	A Density Functional Theory for Symmetric Radical Cations from Bonding to Dissociation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12789-12791.	1.1	45
3242	Origin of Stereoselectivity in the Reduction of a Planar Oxacarbenium. <i>Organic Letters</i> , 2008, 10, 3769-3772.	2.4	23
3243	Accelerating QM/MM Free Energy Calculations: Representing the Surroundings by an Updated Mean Charge Distribution. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5680-5692.	1.2	52
3244	Hierarchical Self-Assembly of Aminopyrazole Peptides into Nanorosettes in Water. <i>Journal of the American Chemical Society</i> , 2008, 130, 586-591.	6.6	20
3245	Theoretical Study of Gallium Nitride Molecules, GaN ₂ and GaN ₄ . <i>Journal of Physical Chemistry A</i> , 2008, 112, 8858-8867.	1.1	3
3246	Accurate Molecular Polarizabilities Based on Continuum Electrostatics. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1480-1493.	2.3	18
3247	Silicon-Carbon Unsaturated Compounds. 75. Thermal Isomerization of 2-Alkyl- and 2-Aryl-2-trimethylsiloxy-1,1-bis(trimethylsilyl)-1-silacyclohex-4-enes. <i>Organometallics</i> , 2008, 27, 2922-2928.	1.1	11
3248	Computational Studies on the Mechanisms and Dynamics of OH Reactions with CHF ₂ CHFOCF ₃ and CHF ₂ CH ₂ OCF ₃ . <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1073-1082.	2.3	14
3249	The Vibrational Spectrum of the Secondary Electron Acceptor, A ₁ , in Photosystem I. <i>Journal of Physical Chemistry B</i> , 2008, 112, 3844-3852.	1.2	7
3250	Benchmark Data for Interactions in Zeolite Model Complexes and Their Use for Assessment and Validation of Electronic Structure Methods. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6860-6868.	1.5	157
3251	Toward a Better Understanding of the Reactivity of Titanium and Zirconium Complexes with an Aryl-Substituted Tripodal Triamido Ligand Derived from cis,cis-1,3,5-Triaminocyclohexane: A Density Functional Study. <i>Organometallics</i> , 2008, 27, 1804-1808.	1.1	0
3252	Dissociation of Acetone Radical Cation (CH ₃ COCH ₃ + \dot{A} \rightarrow CH ₃ CO+ + CH ₃ \dot{A}): An Ab Initio Direct Classical Trajectory Study of the Energy Dependence of the Branching Ratio. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13121-13127.	1.1	14
3253	A Study of the Hydrogen Abstraction Reactions of C ₂ H Radical with CH ₃ CN, C ₂ H ₅ CN, and C ₃ H ₇ CN by Dual-Level Generalized Transition State Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8455-8463.	1.1	4

#	ARTICLE	IF	CITATIONS
3254	Assessment of a Middle-Range Hybrid Functional. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1254-1262.	2.3	155
3255	Where Does the Electron Go? Electron Distribution and Reactivity of Peptide Cation Radicals Formed by Electron Transfer in the Gas phase. <i>Journal of the American Chemical Society</i> , 2008, 130, 8818-8833.	6.6	60
3256	Molecular Dynamics Simulations of H ₂ Adsorption in Tetramethyl Ammonium Lithium Phthalocyanine Crystalline Structures. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15775-15782.	1.2	4
3257	On the Nature of the Intermediates and the Role of Chloride Ions in Pd-Catalyzed Allylic Alkylations: Added Insight from Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12862-12867.	1.1	46
3258	New Insights into the Use of (TD-)DFT for Geometries and Electronic Structures of Constrained π -Stacked Systems: [n.n]Paracyclophanes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13691-13698.	1.1	18
3259	Mixed Alkylamido Aluminate as a Kinetically Controlled Base. <i>Journal of the American Chemical Society</i> , 2008, 130, 16193-16200.	6.6	74
3260	Computational Study of the Gas Phase Reactions of Isopropylimido and Allylimido Tungsten Precursors for Chemical Vapor Deposition of Tungsten Carbonitride Films: Implications for the Choice of Carrier Gas. <i>Chemistry of Materials</i> , 2008, 20, 7246-7251.	3.2	21
3261	Spectroscopic and Computational Insights into Second-Sphere Amino-Acid Tuning of Substrate Analogue/Active-Site Interactions in Iron(III) Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2008, 47, 3993-4004.	1.9	18
3262	Prediction of a New Pathway to Presilphiperfolanol. <i>Organic Letters</i> , 2008, 10, 4827-4830.	2.4	49
3263	Ni ⁺ Reactions with Aminoacrylonitrile, A Species of Potential Astrochemical Relevance. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10509-10515.	1.1	6
3264	Origins of Stereoselectivity in the Oxido-Alkylidenation of Alkynes. <i>Organic Letters</i> , 2008, 10, 4597-4600.	2.4	22
3265	Effect of Substituents on the GPx-like Activity of Ebselen: Steric versus Electronic. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1013-1017.	1.1	41
3266	Theoretical and Experimental Studies of Tyrosyl Hydroperoxide Formation in the Presence of H-Bond Donors. <i>Chemical Research in Toxicology</i> , 2008, 21, 1923-1932.	1.7	10
3267	Benchmarks for electronically excited states: Time-dependent density functional theory and density functional theory based multireference configuration interaction. <i>Journal of Chemical Physics</i> , 2008, 129, 104103.	1.2	478
3268	Inherent Chirality Dominates the Visible/Near-Ultraviolet CD Spectrum of Rhodopsin. <i>Journal of the American Chemical Society</i> , 2008, 130, 6170-6181.	6.6	52
3269	A CASSCF and CASPT2 Study on the Excited States of s-trans-Formaldazine. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8979-8985.	1.1	1
3270	How Important Is the Position of the Molecule between the Electrodes in Tuning Negative Differential Resistance Behavior?. <i>Journal of Physical Chemistry C</i> , 2008, 112, 15537-15542.	1.5	13
3271	Redox Transformations of Bis(2,2'-bipyridine)(1-methyl-1-pyridin-2-yl-ethylamine)ruthenium(II). <i>Inorganic Chemistry</i> , 2008, 47, 5314-5323.	1.9	5

#	ARTICLE	IF	CITATIONS
3272	Quantum Chemical Modeling of Ground States of CO ₂ Chemisorbed on Anatase (001), (101), and (010) TiO ₂ Surfaces. <i>Energy & Fuels</i> , 2008, 22, 2611-2618.	2.5	59
3273	Dependence of Charge-Transport Parameters on Static Correlation and Self-Interaction Energy: The Case of a 1,4-Bis(Phenylethynyl)Benzene Derivative Conjugated Molecule. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10325-10332.	1.1	22
3274	Microhydration of the Guanine-Cytosine (GC) Base Pair in the Neutral and Anionic Radical States: A Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5189-5198.	1.2	48
3275	Synthesis of a Dialuminum-Substituted Silicotungstate and the Diastereoselective Cyclization of Citronellal Derivatives. <i>Journal of the American Chemical Society</i> , 2008, 130, 15872-15878.	6.6	99
3276	Origins of Opposite Syn-Anti Diastereoselectivities in Primary and Secondary Amino Acid-Catalyzed Intermolecular Aldol Reactions Involving Unmodified β -Hydroxyketones. <i>Journal of Organic Chemistry</i> , 2008, 73, 5264-5271.	1.7	15
3277	Large Blue-Shift in the Optical Spectra of Fluorinated Polyphenylenevinylenes. A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2996-3004.	1.2	38
3278	Synthesis and Spin-Trapping Properties of a New Spirolactonyl Nitron. <i>Journal of Organic Chemistry</i> , 2008, 73, 2533-2541.	1.7	26
3279	Tailoring the Metallocene Structure To Obtain LLDPE by Ethene Homopolymerization: An Experimental and Theoretical Study. <i>Organometallics</i> , 2008, 27, 1367-1371.	1.1	7
3280	Experimental Evidence for an Inverse Hydrogen Migration in Arginine Radicals. <i>Journal of the American Chemical Society</i> , 2008, 130, 7645-7654.	6.6	35
3281	Factors Governing Electron Capture by Small Disulfide Loops in Two-Cysteine Peptides. <i>Journal of Physical Chemistry B</i> , 2008, 112, 13661-13669.	1.2	11
3282	Axial Ligand Effects on the Geometric and Electronic Structures of Nonheme Oxoiron(IV) Complexes. <i>Journal of the American Chemical Society</i> , 2008, 130, 12394-12407.	6.6	177
3283	Proton Transfer at Metal Sites in Proteins Studied by Quantum Mechanical Free-Energy Perturbations. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 985-1001.	2.3	40
3284	Semiempirical Double-Hybrid Density Functional with Improved Description of Long-Range Correlation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2702-2712.	1.1	123
3285	Binding to DNA Purine Base and Structure-Activity Relationship of a Series of Structurally Related Ru(II) Antitumor Complexes: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9966-9974.	1.2	20
3286	Dehydrative Cyclocondensation Reactions on Hydrogen-Terminated Si(100) and Si(111): An ex Situ Tool for the Modification of Semiconductor Surfaces. <i>Journal of the American Chemical Society</i> , 2008, 130, 16216-16223.	6.6	34
3287	Electronic, Optical, and Vibrational Properties of Bridged Dithienylethylene-Based NLO Chromophores. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3109-3120.	1.5	48
3288	Quantum Chemistry and Computational Kinetics of the Reaction between OH Radicals and Formaldehyde Adsorbed on Small Silica Aerosol Models. <i>Journal of Physical Chemistry C</i> , 2008, 112, 4590-4600.	1.5	19
3289	Cycloaddition Reactions of Phenylazide and Benzylazide on a Si(100)-2 \times 1 Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 4297-4303.	1.5	21

#	ARTICLE	IF	CITATIONS
3290	Model Potential Approaches for Describing the Interaction of Excess Electrons with Water Clusters: Incorporation of Long-Range Correlation Effects. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11021-11035.	1.1	68
3291	Magnetic Interactions in Alkyl Substituted Cyclohexane Diradical Systems: A Broken Symmetry Approach. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3409-3413.	1.1	7
3292	Hidden Histidine Radical Rearrangements upon Electron Transfer to Gas-Phase Peptide Ions. Experimental Evidence and Theoretical Analysis. <i>Journal of the American Chemical Society</i> , 2008, 130, 14584-14596.	6.6	64
3293	Claisen Rearrangement of Aliphatic Allyl Vinyl Ethers in the Presence of Copper(II) Bisoxazoline. <i>Journal of Organic Chemistry</i> , 2008, 73, 4800-4809.	1.7	13
3294	Theoretical Thermodynamics for Large Molecules: Walking the Thin Line between Accuracy and Computational Cost. <i>Accounts of Chemical Research</i> , 2008, 41, 569-579.	7.6	329
3295	o- and m-Phenylethynyl Radicals and Their Isomers o-, m-, and p-Ethynylphenyl: Structures, Energetics, and Electron Affinities. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2838-2845.	1.1	5
3296	Selective Formation of Rearranged Silenes from Polysilylenones via 1,3- and 1,5-Silyl Migration. <i>Organometallics</i> , 2008, 27, 5423-5425.	1.1	4
3297	Understanding the Behavior of N-Tosyl and N-2-Pyridylsulfonyl Imines in Cu(II)-Catalyzed Aza-Friedel-Crafts Reactions. <i>Journal of Organic Chemistry</i> , 2008, 73, 6401-6404.	1.7	59
3298	Electrochemical, Magnetic, and Electrical Properties of μ_2 -Capped Sexithiophene Films. Part 3. Conduction in Poly(bis-terthienyl-B)s (B = Ethane, Disulfide, Diacetylene, Acetylene, Ethylene). <i>Chemistry of Materials</i> , 2008, 20, 6847-6856.	3.2	12
3299	Decabromobiphenyl (PBB-209) Activates the Aryl Hydrocarbon Receptor While Decachlorobiphenyl (PCB-209) Is Inactive: Experimental Evidence and Computational Rationalization of the Different Behavior of Some Halogenated Biphenyls. <i>Chemical Research in Toxicology</i> , 2008, 21, 643-658.	1.7	19
3300	Reactivity of Superoxide Radical Anion and Hydroperoxyl Radical with μ_2 -Phenyl-N-tert-butyl nitron (PBN) Derivatives. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12498-12509.	1.1	35
3301	Kinetics Study of the OH + Alkene \rightarrow H ₂ O + Alkenyl Reaction Class. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1436-1444.	1.1	20
3302	Photomodulated Chiral Induction in Helical Azobenzene Oligomers. <i>Organic Letters</i> , 2008, 10, 1671-1674.	2.4	51
3303	Formation of Sugar Radicals in RNA Model Systems and Oligomers via Excitation of Guanine Cation Radical. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2168-2178.	1.2	33
3304	Computational Study of the Reaction of C ₆ F ₆ with [IrMe(PEt ₃) ₃]: Identification of a Phosphine-Assisted C ⁺ F Activation Pathway via a Metallophosphorane Intermediate. <i>Journal of the American Chemical Society</i> , 2008, 130, 15490-15498.	6.6	81
3305	Synthesis, X-Ray Crystallographic Characterization, and Electronic Structure Studies of a Di-Azide Iron(III) Complex: Implications for the Azide Adducts of Iron(III) Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2008, 47, 5762-5774.	1.9	8
3306	Chemisorption-induced Structural Changes and Transition from Chemisorption to Physisorption in Au ₆ (CO) _n (n = 4-9). <i>Journal of Physical Chemistry C</i> , 2008, 112, 11920-11928.	1.5	51
3307	Binding Properties of Cu ²⁺ -(glycyl) _n -glycine Complexes (n = 1-19). <i>Journal of Physical Chemistry B</i> , 2008, 112, 11929-11937.	1.1	19

#	ARTICLE	IF	CITATIONS
3308	Theoretical Characterization of a Typical Hole/Exciton-Blocking Material Bathocuproine and Its Analogues. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9097-9103.	1.1	53
3309	Geometries and Stabilities of the Carbon Clusters with the Rhodium Impurity: A Computational Investigation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4375-4381.	1.1	11
3310	Modulation of the Refractive Index by Photoisomerization of Diarylethenes: Theoretical Modeling. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7473-7480.	1.1	22
3311	Structural and Electronic Properties of Crown Ether Functionalized Oligothiophenes. <i>Macromolecules</i> , 2008, 41, 3919-3924.	2.2	8
3312	Mechanism for the Transport of Ammonia within Carbamoyl Phosphate Synthetase Determined by Molecular Dynamics Simulations. <i>Biochemistry</i> , 2008, 47, 2935-2944.	1.2	17
3313	A Quantum Mechanical Study of the Abstraction Reactions of Fused Bicyclic Dimetallenes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10064-10070.	1.1	1
3314	Electronic Structure Studies on Deprotonation of Dithiophosphinic Acids in Water Clusters. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12270-12280.	1.1	8
3315	Ab Initio Density Functional Study on Negative Differential Resistance in a Fused Furan Trimer. <i>Journal of Physical Chemistry C</i> , 2008, 112, 1685-1693.	1.5	43
3316	The Acidity and Proton Affinity of the Damaged Base 1,6-Ethnoadenine in the Gas Phase versus in Solution: Intrinsic Reactivity and Biological Implications. <i>Journal of Organic Chemistry</i> , 2008, 73, 5907-5914.	1.7	34
3317	A Mechanism for the Palladium-Catalyzed Regioselective Silaboration of Allene: A Theoretical Study. <i>Organometallics</i> , 2008, 27, 1736-1742.	1.1	47
3318	Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrroline N-Oxide (DMPO). 3. Effect of Mildly Acidic pH on the Thermodynamics and Kinetics of Adduct Formation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2447-2455.	1.1	30
3319	Biophysical Techniques in Photosynthesis. <i>Advances in Photosynthesis and Respiration</i> , 2008, , .	1.0	21
3320	Dicarbollylamine Ligand as a Tunable Template for σ - and π -Bonding Modes: Syntheses, Structures, and Theoretical Studies of σ -1-Coordinated Constrained-Geometry Group 13 Metal Complexes. <i>Journal of the American Chemical Society</i> , 2008, 130, 9904-9917.	6.6	27
3321	Intersystem Crossing Mediated by Photoinduced Intramolecular Charge Transfer: Anthracene Molecules with Perpendicular π Systems. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4194-4201.	1.1	259
3322	Coordination Properties of Lysine Interacting with Co(I) and Co(II). A Theoretical and Mass Spectrometry Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12385-12392.	1.1	9
3323	Gas-Phase Thermochemical Properties of Pyrimidine Nucleobases. <i>Journal of Organic Chemistry</i> , 2008, 73, 9283-9291.	1.7	59
3324	Conformational Preferences of β^2 - and β^3 -Aminated Proline Analogues. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14045-14055.	1.2	14
3325	Substrate-assisted Catalysis in the Aminoacyl Transfer Mechanism of Histidyl-tRNA Synthetase: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16874-16882.	1.2	24

#	ARTICLE	IF	CITATIONS
3326	The Mechanism for the Rhodium-Catalyzed Decarbonylation of Aldehydes: A Combined Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2008, 130, 5206-5215.	6.6	180
3327	Highly <i>l</i> - and <i>d</i> -enantioselective variants of horseradish peroxidase discovered by an ultrahigh-throughput selection method. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 17694-17699.	3.3	48
3328	Structure and Properties of Molecular Solutes in Electronic Excited States: a Polarizable Continuum Model approach based on the Time-Dependent Density Functional Theory. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008, , 179-208.	0.6	4
3329	DENSITY FUNCTIONAL THEORETICAL STUDY OF MONO-NITRATED FLUORANTHENES. <i>Polycyclic Aromatic Compounds</i> , 2008, 28, 193-212.	1.4	8
3330	Low-lying isomers of the B ₉ boron cluster: The planar molecular wheel versus three-dimensional structures. <i>Journal of Chemical Physics</i> , 2008, 129, 024302.	1.2	82
3331	High-Resolution Spectroscopy of Methyl 4-Hydroxycinnamate and Its Hydrogen-Bonded Water Complex. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4427-4434.	1.2	37
3332	Lactic acid in solution: Investigations of lactic acid self-aggregation and hydrogen bonding interactions with water and methanol using vibrational absorption and vibrational circular dichroism spectroscopies. <i>Journal of Chemical Physics</i> , 2008, 128, 014508.	1.2	95
3333	THEORETICAL STUDY ON SPIN POLARIZATION IN SMALL ALUMINUM CLUSTERS. <i>Journal of Theoretical and Computational Chemistry</i> , 2008, 07, 167-176.	1.8	2
3334	2D/3D-QSAR STUDY ON ANALOGUES OF 2-METHOXYESTRADIOL WITH ANTICANCER ACTIVITY. <i>Journal of Theoretical and Computational Chemistry</i> , 2008, 07, 287-301.	1.8	6
3335	New insight brought by density functional theory on the chemical state of alaninol on Cu(100): Energetics and interpretation of x-ray photoelectron spectroscopy data. <i>Journal of Chemical Physics</i> , 2008, 128, 114709.	1.2	14
3336	Characterization of cyclic and linear C ₃ H ⁺ and C ₃ H via anion photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , 2008, 128, 034301.	1.2	28
3337	Complex polarization propagator calculations of magnetic circular dichroism spectra. <i>Journal of Chemical Physics</i> , 2008, 128, 094103.	1.2	63
3338	Electronic spectrum of TaO and its hyperfine structure. <i>Journal of Chemical Physics</i> , 2008, 128, 104302.	1.2	12
3339	Anion photoelectron spectroscopy of C ₅ H ⁺ . <i>Journal of Chemical Physics</i> , 2008, 128, 174301.	1.2	8
3340	What can we learn from the adiabatic connection formalism about local hybrid functionals?. <i>Journal of Chemical Physics</i> , 2008, 128, 214107.	1.2	44
3341	Characterization of Lewis acid sites on the (100) surface of Î²-AlF ₃ : Ab initio calculations of NH ₃ adsorption. <i>Journal of Chemical Physics</i> , 2008, 128, 224703.	1.2	10
3342	Ab initio study of charge transport of hydrogen functionalized palladium wires. <i>Journal of Chemical Physics</i> , 2008, 129, 024702.	1.2	5
3343	Adiabatic connection forms in density functional theory: H ₂ and the He isoelectronic series. <i>Journal of Chemical Physics</i> , 2008, 129, 064105.	1.2	21

#	ARTICLE	IF	CITATIONS
3344	Density functional localized orbital corrections for transition metals. Journal of Chemical Physics, 2008, 129, 164108.	1.2	42
3345	Controlling spin contamination using constrained density functional theory. Journal of Chemical Physics, 2008, 129, 114110.	1.2	39
3346	Effect of the nonlocal exchange on the performance of the orbital-dependent correlation functionals from second-order perturbation theory. Journal of Chemical Physics, 2008, 129, 124109.	1.2	17
3347	Self-consistent generalized Kohn-Sham local hybrid functionals of screened exchange: Combining local and range-separated hybridization. Journal of Chemical Physics, 2008, 129, 124110.	1.2	68
3348	Theoretical prediction of HRgCO ⁺ ion (Rg=He, Ne, Ar, Kr, and Xe). Journal of Chemical Physics, 2008, 129, 184302.	1.2	37
3349	Localized orbital corrections applied to thermochemical errors in density functional theory: The role of basis set and application to molecular reactions. Journal of Chemical Physics, 2008, 129, 214105.	1.2	19
3350	Delocalization errors in density functionals and implications for main-group thermochemistry. Journal of Chemical Physics, 2008, 129, 204112.	1.2	159
3351	Hartree-Fock orbitals significantly improve the reaction barrier heights predicted by semilocal density functionals. Journal of Chemical Physics, 2008, 128, 244112.	1.2	89
3352	Density functional restricted-unrestricted approach for nonlinear properties: Application to electron paramagnetic resonance parameters of square planar copper complexes. Journal of Chemical Physics, 2008, 129, 064109.	1.2	17
3353	Oligo(vinylidene fluoride) Langmuir-Blodgett films studied by spectroscopic ellipsometry and the density functional theory. Journal of Chemical Physics, 2008, 129, 064704.	1.2	7
3354	Origin of the liquid-liquid phase transition for <i>trans</i> -1,2-dichloroethylene observed by IR spectroscopy. Journal of Chemical Physics, 2008, 129, 074503.	1.2	8
3355	Variational, V-representable, and variable-occupation-number perturbation theories. Journal of Chemical Physics, 2008, 129, 244109.	1.2	8
3356	Geometric and electronic structures of a hole-transport material, TPD, and related materials studied by DFT calculations and solid-state NMR. Proceedings of SPIE, 2008, , .	0.8	1
3357	Combining the hybrid functional method with dynamical mean-field theory. Europhysics Letters, 2008, 84, 57009.	0.7	17
3358	Focusing the view on nature's water-splitting catalyst. Philosophical Transactions of the Royal Society B: Biological Sciences, 2008, 363, 1167-1177.	1.8	60
3359	Excess electron states in reduced bulk anatase TiO ₂ : Comparison of standard GGA, GGA+U, and hybrid DFT calculations. Journal of Chemical Physics, 2008, 129, 154113.	1.2	472
3360	Absorption Enhancement and Conformational Control of Peptides by Small Silver Clusters. Physical Review Letters, 2008, 101, 213001. http://www.w3.org/1998/Math/MathML	2.9	50
3361	display="inline"> <mml:mrow> <mml:mi>PBE</mml:mi> <mml:mo>+</mml:mo> <mml:mi>U</mml:mi> </mml:mrow> </mml:math> calculation of the Jahn-Teller effect in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"> <mml:mrow> <mml:mi mathvariant="normal">Pr</mml:mi> <mml:msub> <mml:mi mathvariant="normal">O</mml:mi> <mml:mn>2</mml:mn> </mml:msub> </mml:mrow> </mml:math>. Physical Review B, 2008, 77, .	1.1	35

#	ARTICLE	IF	CITATIONS
3362	The adsorption of CO on charged and neutral Au and Au ₂ : A comparison between wave-function based and density functional theory. Journal of Chemical Physics, 2008, 128, 124302. $\langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle$	1.2	27
3363	$\display="inline">\langle \text{mml:mi} \rangle \tilde{f} \langle / \text{mml:mi} \rangle \langle / \text{mml:math} \rangle$ -bonding contribution of a strong $\langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle$ $\display="inline">\langle \text{mml:mi} \rangle \tilde{\epsilon} \langle / \text{mml:mi} \rangle \langle / \text{mml:math} \rangle$ -acceptor molecule: Surface chemical bond of $\langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle$ $\display="inline">\langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{SO} \langle / \text{mml:mtext} \rangle \langle / \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 2 \langle / \text{mml:mn} \rangle \langle / \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{LaMnO} \langle / \text{mml:mtext} \rangle \langle / \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle / \text{mml:mn} \rangle \langle / \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{La} \langle / \text{mml:mtext} \rangle \langle / \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 1 \langle / \text{mml:mn} \rangle \langle / \text{mml:mrow} \rangle$	1.1	4
3364	Dielectric properties and excitons for extended systems from hybrid functionals. Physical Review B, 2008, 78, .	1.1	303
3365	V 51 solid-state NMR and density functional theory studies of vanadium environments in V(V)O ₂ dipicolinic acid complexes. Journal of Chemical Physics, 2008, 128, 052317.	1.2	32
3366	Exploring the High Pressure Phase Diagrams of Light Elements Using Large Scale Ab-initio Molecular Dynamics Simulations. 2008 22nd International Symposium on High Performance Computing Systems and Applications, 2008, . $\langle \text{mml:mtext} \rangle \text{Thermodynamic stability of} \langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle$	0.0	0
3367	$\langle \text{mml:mtext} \rangle \text{Thermodynamic stability of} \langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle$ $\langle \text{mml:mtext} \rangle \text{LaMnO} \langle / \text{mml:mtext} \rangle \langle / \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle / \text{mml:mn} \rangle \langle / \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{La} \langle / \text{mml:mtext} \rangle \langle / \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 1 \langle / \text{mml:mn} \rangle \langle / \text{mml:mrow} \rangle$ Physical Review B, 2008, 78	1.1	85
3368	Quantum chemical study of the initial surface reactions of atomic layer deposition GaAs for photonic crystal fabrication. Applied Physics Letters, 2008, 92, .	1.5	6
3369	Electrostatic effects on cluster simulation of ionic crystals and surfaces. Journal of Physics: Conference Series, 2008, 117, 012009.	0.3	0
3371	Electronic Properties of Charge-Tagged Peptides upon Electron Capture. European Journal of Mass Spectrometry, 2008, 14, 367-378.	0.5	10
3372	<i>ortho</i> -Nitrobenzaldehyde 1:1 Water Complexes. The Influence of Solute Water Interactions in the Vertical Excited Spectrum. Zeitschrift Fur Physikalische Chemie, 2008, 222, 1263-1278.	1.4	2
3373	Theoretical Studies on Electronic Structures and Chemical Indices of the Active Site of Oxygenated and Deoxygenated Hemerythrin. Bulletin of the Chemical Society of Japan, 2008, 81, 91-102.	2.0	14
3374	Magnetic Ordering in Organic-Radical Assemblies. Bulletin of the Chemical Society of Japan, 2008, 81, 966-978.	2.0	5
3375	Feasibility of density functional methods to predict dielectric properties of polymers. Journal of Chemical Physics, 2008, 128, 064109.	1.2	7
3376	Parameterized local hybrid functionals from density-matrix similarity metrics. Journal of Chemical Physics, 2008, 128, 084111.	1.2	42
3377	Enhanced Conductance via Induced $\hat{\pi}$ -Stacking Interactions in Cobalt(II) Terpyridine Bridged Complexes. Journal of Physical Chemistry B, 2008, 112, 16070-16075.	1.2	12
3379	Local reactivity of O ₂ with Pt ₃ on Co ₃ Pt and related backgrounds. Journal of Chemical Physics, 2008, 128, 204701.	1.2	7
3380	A DFT Study on Deactivation of Triplet Excited State Riboflavin by Polyphenols. International Journal of Molecular Sciences, 2008, 9, 1908-1914.	1.8	9
3383	Modifying the electronic structure of semiconducting single-walled carbon nanotubes by Ar-ion irradiation. Physical Review B, 2009, 79, .	1.1	42

#	ARTICLE	IF	CITATIONS
3384	Tailoring band gaps of insulators by adsorption at surface defects: Benzoic acids on NaCl surfaces. <i>Physical Review B</i> , 2009, 79, .	1.1	16
3385	Silver Cluster Chromophores for Absorption Enhancement of Peptides. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3783-3788.	1.1	11
3386	Antioxidant Properties of Pterocarpan through Their Copper(II) Coordination Ability. A DFT Study in Vacuo and in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2009, 113, 15206-15216.	1.1	48
3387	Preparation, characterisation and structure of Ti and Al ultrathin oxide films on metals. <i>International Reviews in Physical Chemistry</i> , 2009, 28, 517-576.	0.9	75
3388	Assessment of double-hybrid energy functionals for π -conjugated systems. <i>Journal of Chemical Physics</i> , 2009, 131, 084108.	1.2	74
3389	On the self-consistent implementation of general occupied-orbital dependent exchange-correlation functionals with application to the B05 functional. <i>Journal of Chemical Physics</i> , 2009, 131, 084103.	1.2	25
3390	Role of Si and Ge as impurities in ZnO. <i>Physical Review B</i> , 2009, 80, .	1.1	84
3391	Order- $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:mi} \rangle \text{N} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ implementation of exact exchange in extended insulating systems. <i>Physical Review B</i> , 2009, 79, .	1.1	171
3392	Methane storage in bottle-like nanocapsules. <i>Nanotechnology</i> , 2009, 20, 125602.	1.3	34
3393	Density functional method including weak interactions: Dispersion coefficients based on the local response approximation. <i>Journal of Chemical Physics</i> , 2009, 131, 224104.	1.2	204
3394	A comparative study on the LDA + U and hybrid functional methods on the description of the electronic structure of YTiO ₃ under high pressure. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1374-1382.	0.6	3
3395	Impurity-bound small polarons in ZnO: Hybrid density functional calculations. <i>Physical Review B</i> , 2009, 80, .	1.1	71
3396	Hybrid-functional calculations with plane-wave basis sets: Effect of singularity correction on total energies, energy eigenvalues, and defect energy levels. <i>Physical Review B</i> , 2009, 80, .	1.1	112
3397	Slow photoelectron velocity-map imaging spectroscopy of C ₃ O ⁺ and C ₃ S ⁺ . <i>Journal of Chemical Physics</i> , 2009, 131, 054312.	1.2	8
3398	Defect-induced chemisorption of nitrogen oxides on (10,0) single-walled carbon nanotubes: Insights from density functional calculations. <i>Journal of Chemical Physics</i> , 2009, 131, 114706.	1.2	20
3399	On the origin of ultrafast nonradiative transitions in nitro-polycyclic aromatic hydrocarbons: Excited-state dynamics in 1-nitronaphthalene. <i>Journal of Chemical Physics</i> , 2009, 131, 224518.	1.2	110
3400	<i>Ab initio</i> molecular dynamics calculations of ion hydration free energies. <i>Journal of Chemical Physics</i> , 2009, 130, 204507.	1.2	111
3401	Mild template synthesis in the iron(III)-ethanedithioamide-1,2-formaldehyde triple system on a K[Fe(CN) ₆] gelatin-immobilized matrix. <i>Journal of Coordination Chemistry</i> , 2009, 62, 1058-1066.	0.8	10

#	ARTICLE	IF	CITATIONS
3402	A relook at the compliance constants in redundant internal coordinates and some new insights. Journal of Chemical Physics, 2009, 131, 174112.	1.2	25
3403	Insights into the Maillard reaction. The mechanism of Schiff's base formation from the reaction force perspective. Molecular Physics, 2009, 107, 1587-1596.	0.8	6
3404	SOLVENT AND SUBSTITUENT EFFECTS ON THE INTRAMOLECULAR AMIDE HYDROLYSIS OF N-METHYLMALEAMIC ACID. Journal of Theoretical and Computational Chemistry, 2009, 08, 1217-1226.	1.8	1
3405	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
3406	THE INFLUENCES OF OXIDATION AND CATIONIZATION ON THE N-GLYCOSIDIC BOND STABILITY OF 8-OXO-2-DEOXYADENOSINE A THEORETICAL STUDY. Journal of Theoretical and Computational Chemistry, 2009, 08, 1253-1264.	1.8	6
3407	AB INITIO INVESTIGATION OF ELECTRONIC AND VIBRATIONAL PROPERTIES OF ZnS AND ZnSe CRYSTALS BY DIFFERENT XC-FUNCTIONALS. International Journal of Modern Physics B, 2009, 23, 3845-3857.	1.0	6
3409	What Differs on the Enzymatic Acetylation Mechanisms for Arylamines and Arylhydrazines Substrates? A Theoretical Study. Research Letters in Biochemistry, 2009, 2009, 1-5.	0.0	0
3410	Post-CCSD(T) ab Initio Thermochemistry of Halogen Oxides and Related Hydrides XO, XOO, HOX, XO _n , and HXO _n (X = F, Cl), and Evaluation of DFT Methods for These Systems. Journal of Physical Chemistry A, 2009, 113, 4802-4816.	1.1	77
3411	Effect of lattice topology on the adsorption of benzyl alcohol on kaolinite surfaces: Quantum chemical calculations of geometry optimization, binding energy, and NMR chemical shielding. American Mineralogist, 2009, 94, 1392-1404.	0.9	14
3412	Force field for the atomistic simulation of the properties of hydrazine, organic hydrazine derivatives, and energetic hydrazinium ionic liquids. Pure and Applied Chemistry, 2009, 81, 1799-1828.	0.9	30
3413	Growth and Material Characterization of Hafnium Titanates Deposited by Atomic Layer Deposition. Journal of the Electrochemical Society, 2009, 156, G145.	1.3	15
3414	Modeling two photon absorption cross sections of open-shell systems. Journal of Chemical Physics, 2009, 130, 014103.	1.2	8
3415	Representation independent algorithms for molecular response calculations in time-dependent self-consistent field theories. Journal of Chemical Physics, 2009, 130, 054111.	1.2	92
3416	Coupled-cluster and density functional theory studies of the electronic excitation spectra of trans-1,3-butadiene and trans-2-propeniminium. Journal of Chemical Physics, 2009, 131, 024301.	1.2	44
3417	Local hybrids as a perturbation to global hybrid functionals. Journal of Chemical Physics, 2009, 131, 154112.	1.2	33
3418	A comparative study of hydrogen-atom release dynamics in radical-radical reactions. Physica Scripta, 2009, 80, 048116.	1.2	0
3419	Proton momentum distribution and anomalous scattering intensities in a pseudo-spherical ammonium ion: a neutron Compton scattering study of (NH ₄) ₂ PdCl ₆ and (NH ₄) ₂ TeCl ₆ . Journal of Physics Condensed Matter, 2009, 21, 075502.	0.7	2
3420	CS Activation of CS ₂ by Nb ⁺ in Gas Phase. Chinese Journal of Chemical Physics, 2009, 22, 297-302.	0.6	0

#	ARTICLE	IF	CITATIONS
3421	Theoretical Study on Reactions of Triplet Excited State Thioxanthone with Indole. <i>International Journal of Molecular Sciences</i> , 2009, 10, 4284-4289.	1.8	9
3422	Density Functional Study of Structures and Electron Affinities of BrO ₄ F/BrO ₄ F ⁻ . <i>International Journal of Molecular Sciences</i> , 2009, 10, 3128-3148.	1.8	1
3423	Design of Carborane Molecular Architectures via Electronic Structure Computations. <i>International Journal of Photoenergy</i> , 2009, 2009, 1-9.	1.4	13
3424	Slow photoelectron velocity-map imaging spectroscopy of C ₂ N ⁺ , C ₄ N ⁺ , and C ₆ N ⁺ . <i>Journal of Chemical Physics</i> , 2009, 130, 064304.	1.2	41
3425	Numerical evaluation of electron repulsion integrals for pseudoatomic orbitals and their derivatives. <i>Journal of Chemical Physics</i> , 2009, 130, 124114.	1.2	13
3426	Interplay between magnetic, electronic, and vibrational effects in monolayer Mn ₃ O ₄ grown on Pd(100). <i>Journal of Chemical Physics</i> , 2009, 130, 124707.	1.2	32
3427	Calculating electron paramagnetic resonance g-matrices for triplet state molecules from multireference spin-orbit configuration interaction wave functions. <i>Journal of Chemical Physics</i> , 2009, 130, 154106.	1.2	14
3428	Full-electron calculation of effective electronic couplings and excitation energies of charge transfer states: Application to hole transfer in DNA π -stacks. <i>Journal of Chemical Physics</i> , 2009, 131, 114113.	1.2	33
3429	Linear and nonlinear optical properties of a series of Ni-dithiolene derivatives. <i>Journal of Chemical Physics</i> , 2009, 131, 134312.	1.2	50
3430	A First Principle Analysis of the Structure of Oligoanilines Doped with Alkylsulfonic Acids. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8795-8800.	1.1	20
3431	A DFT study of the reactions of O ₃ with Hg ⁺ or Br ⁺ . <i>Atmospheric Environment</i> , 2009, 43, 5708-5711.	1.9	12
3432	Replacement of chlorophyll with di-vinyl chlorophyll in the antenna and reaction center complexes of the cyanobacterium <i>Synechocystis</i> sp. PCC 6803: Characterization of spectral and photochemical properties. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2009, 1787, 191-200.	0.5	22
3434	Ambipolar Organic Field-Effect Transistors from Cross-Conjugated Aromatic Quaterthiophenes; Comparisons with Quinoidal Parent Materials. <i>Advanced Functional Materials</i> , 2009, 19, 386-394.	7.8	71
3435	Assignment of the absolute configuration of zwitterionic and neutral macropodumines by means of TDDFT CD calculations. <i>Chirality</i> , 2009, 21, 561-568.	1.3	20
3436	Absolute structural elucidation of natural products—A focus on quantum-mechanical calculations of solid-state CD spectra. <i>Chirality</i> , 2009, 21, E181-201.	1.3	102
3437	Comparative Analysis of Electron-Density and Electron-Localization Function for Dinuclear Manganese Complexes with Bridging Boron- and Carbon-Centered Ligands. <i>Chemistry - A European Journal</i> , 2009, 15, 623-632.	1.7	38
3438	The Effect of a Complexed Lithium Cation on a Norcaradiene-Based Radical Clock. <i>Chemistry - A European Journal</i> , 2009, 15, 2425-2433.	1.7	7
3439	Ferrocenyl-Ended Thieno-Vinylene Oligomers: Donor-Acceptor Polarization and Mixed-Valence Properties with Emphasis on the Raman Mapping of Localized-to-Localized Transitions. <i>Chemistry - A European Journal</i> , 2009, 15, 2548-2559.	1.7	19

#	ARTICLE	IF	CITATIONS
3440	Sensing Abilities of Crown Ether Functionalized Polythiophenes. <i>Chemistry - A European Journal</i> , 2009, 15, 4676-4684.	1.7	13
3441	Hydrogen-Atom Transfer in Reactions of Organic Radicals with [Co ^{II} (por)] ⁺ (por=Porphyrinato) and in Subsequent Addition of [Co(H)(por)] to Olefins. <i>Chemistry - A European Journal</i> , 2009, 15, 4312-4320.	1.7	66
3442	Determination of the Catalytic Pathway of a Manganese Arginase Enzyme Through Density Functional Investigation. <i>Chemistry - A European Journal</i> , 2009, 15, 8026-8036.	1.7	23
3443	Mechanism of Pd(OAc) ₂ /Pyridine Catalyst Reoxidation by O ₂ : Influence of Labile Monodentate Ligands and Identification of a Biomimetic Mechanism for O ₂ Activation. <i>Chemistry - A European Journal</i> , 2009, 15, 2915-2922.	1.7	101
3444	Theoretical Study on the Halogen-Zinc Exchange Reaction by Using Organozincate Compounds. <i>Chemistry - A European Journal</i> , 2009, 15, 5686-5694.	1.7	18
3445	Thiophene-Diazine Molecular Semiconductors: Synthesis, Structural, Electrochemical, Optical, and Electronic Structural Properties; Implementation in Organic Field-Effect Transistors. <i>Chemistry - A European Journal</i> , 2009, 15, 5023-5039.	1.7	82
3446	Cr(CO) ₃ -Activated Diels-Alder Reaction on Single-Wall Carbon Nanotubes: A DFT Investigation. <i>Chemistry - A European Journal</i> , 2009, 15, 4182-4189.	1.7	8
3447	Thermally Stable Solids Based on Endohedrally Doped ZnS Clusters. <i>Chemistry - A European Journal</i> , 2009, 15, 5138-5144.	1.7	19
3448	Emissive or Nonemissive? A Theoretical Analysis of the Phosphorescence Efficiencies of Cyclometalated Platinum(II) Complexes. <i>Chemistry - A European Journal</i> , 2009, 15, 7225-7237.	1.7	198
3449	Lewis Acid Controlled Regioselectivity in Styrene Hydrocyanation. <i>Chemistry - A European Journal</i> , 2009, 15, 8768-8778.	1.7	29
3450	The Controlled Formation and Cleavage of an Intramolecular d ⁸ -d ⁸ Pt-Pt Interaction in a Dinuclear Cycloplatinated Molecular Pivotal Hinge. <i>Chemistry - A European Journal</i> , 2009, 15, 7689-7697.	1.7	23
3451	High-Performance <i>ip</i> -Channel Organic Semiconducting Candidates Based on Benzo[1,2- <i>ik</i> ;4,5- <i>ik</i>]-difluoranthene Derivatives. <i>Chemistry - A European Journal</i> , 2009, 15, 5896-5900.	1.7	12
3452	Oxidation of End-Capped Pentathienoacenes and Characterization of Their Radical Cations. <i>Chemistry - A European Journal</i> , 2009, 15, 12346-12361.	1.7	17
3453	Experimental and Theoretical Study of Tunable 1,3-Lithium Shift of Propargylic/Allenlyic Species, Transmetalation, and Pd-Catalyzed Cross-Coupling Reactions. <i>Chemistry - A European Journal</i> , 2009, 15, 11361-11372.	1.7	36
3454	Synthesis and EPR Studies of 2-Deoxyuridines with Alkynyl, Rodlike Linkages. <i>Chemistry - A European Journal</i> , 2009, 15, 7569-7577.	1.7	15
3455	Synthesis, Structure, and Bonding of Novel Homodinuclear Cobalt and Nickel Borylene Complexes. <i>Chemistry - A European Journal</i> , 2009, 15, 7150-7155.	1.7	11
3456	Synthesis, Spectroscopy, Nonlinear Optics, and Theoretical Investigations of Thienylethynyl Octopoles with a Tunable Core. <i>Chemistry - A European Journal</i> , 2009, 15, 8223-8234.	1.7	14
3457	Vicinal Dinitridoruthenium-Substituted Polyoxometalates [XW ₁₀ O ₃₈ {RuN} ₂] ⁶⁻ (X=Si or Ge). <i>Chemistry - A European Journal</i> , 2009, 15, 10233-10243.	1.7	33

#	ARTICLE	IF	CITATIONS
3458	Ligand-Centred Reactivity of Bis(picoly)amine Iridium: Sequential Deprotonation, Oxidation and Oxygenation of a Non-Innocent Ligand. <i>Chemistry - A European Journal</i> , 2009, 15, 11878-11889.	1.7	60
3459	Enhanced Reactivities of Iron(IV)-Oxo Porphyrin Cation Radicals in Oxygenation Reactions by Electron-Donating Axial Ligands. <i>Chemistry - A European Journal</i> , 2009, 15, 10039-10046.	1.7	110
3460	Geminal Ionic Liquids: A Combined Approach to Investigate Their Three-Dimensional Organisation. <i>Chemistry - A European Journal</i> , 2009, 15, 13059-13068.	1.7	27
3461	Rigid Alicyclic Molecules from Bicyclo[2.2.1]heptanes (=8,9,10-Trinorbornenes) and 1,4-Dipyridinylphthalazines as Stereoselective Coupling Agents. <i>Helvetica Chimica Acta</i> , 2009, 92, 298-312.	1.0	12
3462	Experimental and Theoretical Analyses of Complex Bis[2,4-diphenyl-1,3,5-triazapentadienato]Cu(II) Synthesized <i>in situ</i> . <i>Chinese Journal of Chemistry</i> , 2009, 27, 602-606.	2.6	1
3463	Investigation on the Scavenging Mechanism of 1,4-Dicarbonyls by Pyridoxamine: A Density Functional Theory Study. <i>Chinese Journal of Chemistry</i> , 2009, 27, 1452-1458.	2.6	1
3464	Spin Multiplicity Dependence of Nonlinear Optical Properties. <i>ChemPhysChem</i> , 2009, 10, 817-823.	1.0	27
3465	FT Raman and DFT Study on a Series of All-anti Oligothienoacenes End-Capped with Triisopropylsilyl Groups. <i>ChemPhysChem</i> , 2009, 10, 3069-3076.	1.0	11
3466	A High Molecular Weight Donor for Electron Injection Interlayers on Metal Electrodes. <i>ChemPhysChem</i> , 2009, 10, 2947-2954.	1.0	16
3467	Computational Study of the C- and N-Bound Tautomers of [Ru(Cl)(H)(CO)(PPh ₃) ₂ (I-PrMe ₂)] (I-PrMe ₂ = 3-isopropyl-5-dimethylimidazol-2-ylidene). <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 2000-2006.	1.0	22
3468	Conformational Effects on Long-Range Electron Transfer: Comparison of Oligo-phenylene and Oligo-xylylene Bridges. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 3778-3790.	1.0	60
3469	A Dinuclear Double-Stranded Oxido Complex of ReV with a Bis(benzene-o-dithiolato) Ligand. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 4043-4051.	1.0	19
3470	Pseudoanguilosporin A and B: Two New Isochromans Isolated from the Endophytic Fungus <i>Pseudoanguilospora</i> sp.. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 1427-1434.	1.2	44
3471	The Assignment of Absolute Stereostructures through Quantum Chemical Circular Dichroism Calculations. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 2717-2727.	1.2	295
3472	Controlling Selectivity for Cycloadditions of Nitrones and Alkenes Tethered by Benzimidazoles: Combining Experiment and Theory. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 1578-1584.	1.2	10
3473	Synthesis and Photophysical Characterisation of Fluorescent 8-(1,2,3-triazol-4-yl)adenosine Derivatives. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 1515-1521.	1.2	48
3474	Intramolecular Nonbonded Interactions Between Divalent Selenium Centers with Donor and Acceptor Substituents. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 2765-2774.	1.2	17
3475	New Chiral Lewis Bases Derived from L-Pipecolinic Acid Showing Stereocontrol Highly Dependent on the Catalyst Design in the Hydrosilylation of N-Phenyl Ketimines. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 3357-3367.	1.2	16

#	ARTICLE	IF	CITATIONS
3476	Theoretical studies of the reactions of $\text{CF}_3\text{CHClOCHF}_2/\text{CF}_3\text{CHFOCHF}_2$ with OH radical and Cl atom and their product radicals with OH. <i>Journal of Computational Chemistry</i> , 2009, 30, 565-580.	1.5	20
3477	Comparison of some representative density functional theory and wave function theory methods for the studies of amino acids. <i>Journal of Computational Chemistry</i> , 2009, 30, 589-600.	1.5	61
3478	Dual-level direct dynamics studies for the reactions of OH radical with bromine-substituted ethanes. <i>Journal of Computational Chemistry</i> , 2009, 30, 611-620.	1.5	2
3479	Can the hybrid meta GGA and DFT methods describe the stacking interactions in conjugated polymers?. <i>Journal of Computational Chemistry</i> , 2009, 30, 1179-1184.	1.5	15
3480	Chemical bonding in view of electron charge density and kinetic energy density descriptors. <i>Journal of Computational Chemistry</i> , 2009, 30, 1093-1102.	1.5	62
3481	<i>Ab initio</i> description of photoabsorption and electron transfer in a doubly-linked porphyrin-fullerene dyad. <i>Journal of Computational Chemistry</i> , 2009, 30, 1194-1201.	1.5	8
3482	Typical aromatic noncovalent interactions in proteins: A theoretical study using phenylalanine. <i>Journal of Computational Chemistry</i> , 2009, 30, 1392-1404.	1.5	46
3483	Modeling the H bond donor strength of X_2OH , X_2NH , and X_2CH sites by local molecular parameters. <i>Journal of Computational Chemistry</i> , 2009, 30, 1454-1464.	1.5	39
3484	<i>Ab initio</i> theory for treating local electron excitations in molecules and its performance for computing optical properties. <i>Journal of Computational Chemistry</i> , 2009, 30, 2213-2230.	1.5	18
3485	Substituent effect on electron affinity, gas-phase basicity, and structure of monosubstituted propynyl radicals and their anions: A theoretical study. <i>Journal of Computational Chemistry</i> , 2009, 30, 2181-2186.	1.5	3
3486	$\text{CH}_3\text{NHNH}_2 + \text{OH}$ reaction: Mechanism and dynamics studies. <i>Journal of Computational Chemistry</i> , 2009, 30, 2194-2204.	1.5	15
3487	Modified regional self-interaction corrected time-dependent density functional theory for core excited-state calculations. <i>Journal of Computational Chemistry</i> , 2009, 30, 2583-2593.	1.5	5
3488	Extension of QM/MM docking and its applications to metalloproteins. <i>Journal of Computational Chemistry</i> , 2009, 30, 2609-2616.	1.5	62
3489	Trends of the bonding effect on the performance of DFT methods in electric properties calculations: A pattern recognition and metric space approach on some XY_2 ($\text{X} = \text{O}, \text{S}$ and $\text{Y} = \text{H}, \text{O}, \text{F}, \text{S}$). <i>Tj ETQq1 1.0.7843 14 rgBT /Ov</i>	1.5	14
3490	Rate coefficients for the reaction of OH with $\text{CF}_3\text{CH}_2\text{CH}_3$ (HFC-263fb) between 200 and 400 K: <i>Ab initio</i> , DFT, and transition state theory calculations. <i>Journal of Computational Chemistry</i> , 2010, 31, 500-509.	1.5	9
3491	Covalent hydration energies for purine analogs by quantum chemical methods. <i>Journal of Computational Chemistry</i> , 2010, 31, 721-725.	1.5	6
3492	Using electronic polarization from the internal continuum (EPIC) for intermolecular interactions. <i>Journal of Computational Chemistry</i> , 2010, 31, 811-824.	1.5	8
3493	Pharmacophore mapping and electronic feature analysis for a series of nitroaromatic compounds with antitubercular activity. <i>Journal of Computational Chemistry</i> , 2010, 31, 739-751.	1.5	26

#	ARTICLE	IF	CITATIONS
3494	Evaluation of exchange-correlation functionals for time-dependent density functional theory calculations on metal complexes. <i>Journal of Computational Chemistry</i> , 2010, 31, 1008-1014.	1.5	27
3495	QM/MM study of the absorption spectra of DsRed.M1 chromophores. <i>Journal of Computational Chemistry</i> , 2010, 31, 1603-1612.	1.5	30
3496	Theoretical investigation of the inhibition of corrosion by some triazole Schiff bases. <i>Materials and Corrosion - Werkstoffe Und Korrosion</i> , 2009, 60, 813-819.	0.8	44
3497	Reaction diastereoselectivity of chiral aminoalcohols/[Co(II)NO ₃] ⁺ complexes in evaporating ESI nanodroplets: new insights from a joint experimental and computational investigation. <i>Journal of Mass Spectrometry</i> , 2009, 44, 1038-1046.	0.7	5
3498	Identification and characterisation of the E951 artificial food sweetener by vibrational spectroscopy and theoretical modelling. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 2144-2154.	1.2	20
3500	Gas-Phase Synthesis and Intense Visible Absorption of Tryptophan-Gold Cations. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 7829-7832.	7.2	20
3501	Influence of the dye presence on the conformational preferences of CREKA, a tumor homing linear pentapeptide. <i>Biopolymers</i> , 2009, 92, 83-93.	1.2	17
3502	QM/MM investigation into binding of square-planar platinum complexes to DNA fragments. <i>Journal of Biological Inorganic Chemistry</i> , 2009, 14, 1165-1174.	1.1	23
3503	Theoretical study on the ground state intramolecular proton transfer (IPT) and solvation effect in two Schiff bases formed by 2-aminopyridine with 2-hydroxy-1-naphthaldehyde and 2-hydroxy salicylaldehyde. <i>Journal of Molecular Modeling</i> , 2009, 15, 223-232.	0.8	50
3504	Systematic characterization on electronic structures and spectra for a series of complexes, M(IDB)Cl ₂ (M = Mn, Fe, Co, Ni, Cu and Zn): a theoretical study. <i>Journal of Molecular Modeling</i> , 2009, 15, 469-479.	0.8	10
3505	Performance of Becke's half-and-half functional for non-covalent interactions: energetics, geometries and electron densities. <i>Journal of Molecular Modeling</i> , 2009, 15, 1051-1060.	0.8	17
3506	Towards the design of Cyclooxygenase (COX) inhibitors based on 4,5 di-substituted biphenyl acetic acid molecules: a QSAR study with a new DFT based descriptor - nucleus independent chemical shift. <i>Journal of Molecular Modeling</i> , 2009, 15, 1221-1228.	0.8	8
3507	Study of the structural and electronic origin of the sandalwood odor of some terpenylcyclohexanols. <i>Monatshefte für Chemie</i> , 2009, 140, 1447-1452.	0.9	2
3508	Quantum chemical CD calculations of dioncophylline A in the solid state. <i>Tetrahedron</i> , 2009, 65, 5720-5728.	1.0	37
3509	The mechanism of enantioselective control of an organocatalyst with central and axial chiral elements. <i>Tetrahedron: Asymmetry</i> , 2009, 20, 1365-1368.	1.8	24
3510	Carbocation rearrangements in aspernomine biosynthesis. <i>Tetrahedron Letters</i> , 2009, 50, 1578-1581.	0.7	15
3511	A theoretical insight into the deactivating reactions of triplet excited state C60 by β -carotene. <i>Computational and Theoretical Chemistry</i> , 2009, 893, 111-113.	1.5	1
3512	Direct dynamics studies for the reactions of CH ₃ CH ₂ Br with O (3P) and Cl (2P) atoms. <i>Computational and Theoretical Chemistry</i> , 2009, 897, 36-41.	1.5	3

#	ARTICLE	IF	CITATIONS
3513	Structure-â€˜mutagenicity relationships and energies of 1-, and 2-nitrotriphenylenes. Computational and Theoretical Chemistry, 2009, 899, 79-85.	1.5	7
3514	Reduction of N2O by H2 catalyzed by platinum monocation: A theoretical study. Computational and Theoretical Chemistry, 2009, 902, 109-113.	1.5	3
3515	C-â€˜ versus C-H bond activation of propyne by Y: A DFT study. Computational and Theoretical Chemistry, 2009, 907, 119-125.	1.5	3
3516	The association of dehydro-epiandrosterone and adenosine triphosphate acid: A DFT study of interactions between prototypic biologically active molecules. Computational and Theoretical Chemistry, 2009, 912, 32-37.	1.5	2
3517	Theoretical investigation on the reaction of N2O and CO catalyzed by Fe+(C6H6). Computational and Theoretical Chemistry, 2009, 910, 136-140.	1.5	0
3518	Theoretical study of the scavenging mechanism to 1,4-dicarbonyls by pyridoxamine: The water-assisted reaction. Computational and Theoretical Chemistry, 2009, 911, 70-74.	1.5	4
3519	A DFT study on the mechanism of the gas phase reaction of ground-state Y (4d15s2,2D) with 2-butyne. Computational and Theoretical Chemistry, 2009, 915, 105-111.	1.5	7
3520	First principles study on the properties of p-type conducting In:SnO2. Thin Solid Films, 2009, 517, 3345-3349.	0.8	38
3521	Degradation of the N,N-â€˜bis-(1-naphthyl)-N,â€˜-diphenyl-1,1-â€˜biphenyl-4,4-â€˜diamine by photon irradiation. Thin Solid Films, 2009, 517, 4461-4463.	0.8	6
3522	Relativistic two-component calculations of electronic g-tensor for oxo-molybdenum(V) and oxo-tungsten(V) complexes: The important role of higher-order spin-orbit contributions. Chemical Physics, 2009, 356, 229-235.	0.9	23
3523	Assaying phenothiazine derivatives as trypanothione reductase and glutathione reductase inhibitors by theoretical docking and Molecular Dynamics studies. Journal of Molecular Graphics and Modelling, 2009, 28, 371-381.	1.3	18
3524	Hydrogen bonding. Part 87: DFT MO study of hydration of tetramethyl- and tetraethylammonium ions â€˜ Correlation of hydrate symmetry with 14N to CH NMR coupling. Journal of Molecular Structure, 2009, 919, 117-121.	1.8	1
3525	9-[(Mesityloxy)carbonyl]-10-methylacridinium trifluoromethanesulphonate and its derivative mesityl 9-methoxy-10-methyl-9,10-dihydroacridine-9-carboxylate: Structural and physicochemical features. Journal of Molecular Structure, 2009, 920, 231-237.	1.8	6
3526	Synthesis and conformational analysis of naphthyl-naphthoxazine derivatives. Journal of Molecular Structure, 2009, 929, 58-66.	1.8	5
3527	Probing the adsorption mechanism in thiamazole bound to the silver surface with Surface-enhanced Raman Scattering and DFT. Chemical Physics Letters, 2009, 479, 248-254.	1.2	23
3528	How does microhydration impact on structure, spectroscopy and formation of disulfide radical anions? An ab initio investigation on dimethyldisulfide. Chemical Physics Letters, 2009, 481, 173-179.	1.2	8
3529	Novel meso-substituted porphyrins: Synthesis, characterization and photocatalytic activity of their TiO2-based composites. Dyes and Pigments, 2009, 80, 321-328.	2.0	70
3530	Solvent effect on the thermodynamics of Ag(I) coordination to tripodal polypyridine ligands. Journal of Thermal Analysis and Calorimetry, 2009, 97, 845-851.	2.0	6

#	ARTICLE	IF	CITATIONS
3531	Density functional theory. <i>Photosynthesis Research</i> , 2009, 102, 443-453.	1.6	282
3532	Testing the performance of density functionals for the calculation of energetic properties of complex-forming radical-molecule reactions. <i>Reaction Kinetics and Catalysis Letters</i> , 2009, 96, 233-244.	0.6	4
3533	An ab initio and density functional theory study on the mechanism for the reaction of OH with 2-ethylfuran. <i>Structural Chemistry</i> , 2009, 20, 525-532.	1.0	15
3534	Effects of substituent on the DNA-binding of ruthenium(II) complexes containing asymmetric tridentate intercalative ligands. <i>Transition Metal Chemistry</i> , 2009, 34, 297-305.	0.7	12
3535	Structural and Kinetic DFT Characterization of Materials to Rationalize Catalytic Performance. <i>Topics in Catalysis</i> , 2009, 52, 444-455.	1.3	11
3536	Crystal Structure of Ethyl (2Z, 5R)-2-benzylidene-7-methyl-3-oxo-5-phenyl-2,3-dihydro-5H-[1,3] Thiazolo [3,2-a] Pyrimidine-6-carboxylate. <i>Journal of Chemical Crystallography</i> , 2009, 39, 898-901.	0.5	8
3537	Ab Initio quantum chemical calculation of the structures of coordination compounds arising at template synthesis in ion M(II)-hydrozinomethane thiohydrazide-acetone (M = Co, Ni, Cu) systems. <i>Journal of Structural Chemistry</i> , 2009, 50, 613-617.	0.3	10
3538	From Hartreeâ€Fock and Heitlerâ€London to chemical orbitals. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 209-235.	0.5	7
3539	Density functional methods in the study of oxygen transfer reactions. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 59-66.	0.5	3
3540	The self-interaction error and the description of non-dynamic electron correlation in density functional theory. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 171-182.	0.5	51
3541	Structural and electronic properties of small platinum metallorganic complexes. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 317-325.	0.5	7
3542	Electronic structure and optical properties of chelating heteroatomic conjugated molecules: a SAC-CI study. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 395-408.	0.5	4
3543	Formation of pyrazolâ€1,3,4â€thiadiazoles through 1,3â€dipolar cycloadditions of 3â€thioxoâ€[1,2,4]â€triazepinâ€5â€one with nitrilimines: an experimental and computational study. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 31-41.	0.9	8
3544	Substituent effect on electron affinity, gasâ€phase basicity, and structure of monosubstituted propargyl radicals and their anions: a theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 91-95.	0.9	3
3545	Fragmentation pathways of some benzothiophene radical cations formed by atmospheric pressure chemical ionisation. <i>Rapid Communications in Mass Spectrometry</i> , 2009, 23, 571-579.	0.7	16
3546	The structures, thermochemistry, and electron affinities of hydrogenated silicon clusters Si₆H_n (n = 14). <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1283-1301.	1.0	9
3547	Conclusive evidence on the insensitivity of additive rules to the combinational details of exchange and correlation functional in hybrid DFT methods. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 160-170.	1.0	2
3548	Theoretical study on structures and stabilities of N₄X (X = O, S, Se, Te) series. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 226-235.	1.0	12

#	ARTICLE	IF	CITATIONS
3549	Locally range-separated hybrids as linear combinations of range-separated local hybrids. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2023-2032.	1.0	28
3550	Estimation of effective exchange integral value of polyradical systems based on the band calculation. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3632-3640.	1.0	5
3551	Quantum chemical topology: The electronic structure of the alkaline nitrites MONO (M = Li, Na, K) studied by means of topological analysis of the electron localization function. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1890-1900.	1.0	0
3552	A potential energy surface bifurcation in terpene biosynthesis. <i>Nature Chemistry</i> , 2009, 1, 384-389.	6.6	109
3553	Quantum chemical calculation of the catalytic reaction of ethane dehydrogenation on gallium oxide-hydroxide binuclear clusters in oxidized GaO/ZSM-5 zeolite. <i>Kinetics and Catalysis</i> , 2009, 50, 752-759.	0.3	6
3554	Theoretical studies of stereoselectivities in the direct anti-Mannich and syn-aldol reactions catalyzed by axially chiral amino sulfonamide. <i>Journal of Molecular Catalysis A</i> , 2009, 314, 1-9.	4.8	7
3555	X-ray crystallographic study of 3-Oxo-2-[[4-(thiazol-2-ylsulfamoyl)-phenyl]-hydrazono]-butyric acid ethyl ester and its application in the solvent assisted naked eye sensing of Hg(II). <i>Journal of Molecular Structure</i> , 2009, 927, 60-68.	1.8	12
3556	Stability and molecular dynamics of solid lasamide (API of diuretic and antiviral drugs) studied by ¹ H NMR spectroscopy and DFT methods. <i>Journal of Molecular Structure</i> , 2009, 931, 94-99.	1.8	5
3557	Electronic and magnetic properties of double perovskites (, Ca). <i>Physica B: Condensed Matter</i> , 2009, 404, 2754-2756.	1.3	4
3558	Calibration of computationally predicted N 1s binding energies by comparison with X-ray photoelectron spectroscopy measurements. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2009, 175, 31-40.	0.8	60
3559	Characterization and properties of a polythiophene with a malonic acid dimethyl ester side group. <i>European Polymer Journal</i> , 2009, 45, 2211-2221.	2.6	25
3560	Effect of ancillary ligands on the photophysical properties of Ru(II) complexes bearing a highly conjugated diimine ligand: A density functional theory study. <i>Inorganica Chimica Acta</i> , 2009, 362, 5064-5072.	1.2	10
3561	A new route to thiopyran S,S-dioxide derivatives via an overall ring-enlargement protocol from 3-nitrothiophene. <i>Tetrahedron</i> , 2009, 65, 336-343.	1.0	18
3562	Density functional theory rationalization of the substituent effects in trifluoromethyl-pyridinol derivatives. <i>Tetrahedron</i> , 2009, 65, 232-239.	1.0	17
3563	Chiral Brønsted acid-catalyzed hydrophosphonylation of imines—DFT study on the effect of substituents of phosphoric acid. <i>Tetrahedron</i> , 2009, 65, 4950-4956.	1.0	69
3564	The oxyheme complexes of P450cam: A QM/MM study. <i>Computational and Theoretical Chemistry</i> , 2009, 898, 90-96.	1.5	23
3565	Designing new free-radical reducing reagents: Theoretical study on Si—H bond dissociation energies of organic silanes. <i>Computational and Theoretical Chemistry</i> , 2009, 893, 67-72.	1.5	16
3566	Elimination of HF from CH ₃ F by As ⁺ and Bi ⁺ : A comparative theoretical study. <i>Computational and Theoretical Chemistry</i> , 2009, 894, 36-40.	1.5	2

#	ARTICLE	IF	CITATIONS
3567	Theoretical study of the molecular properties of methyl 2-azidopropionate and methyl 3-azidopropionate. <i>Computational and Theoretical Chemistry</i> , 2009, 894, 80-87.	1.5	2
3568	Anharmonic vibrational analysis of uracil by ab initio Hartree-Fock and density functional theory calculations. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 18-20.	1.5	9
3569	Dehydrohalogenation versus dehydrogenation in reaction of Au ⁺ with CH ₃ Cl: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2009, 899, 18-24.	1.5	12
3570	Effect of water molecules on the decarboxylation of Orotidine 5'-monophosphate catalyzed by Orotidine 5'-monophosphate decarboxylase. <i>Computational and Theoretical Chemistry</i> , 2009, 897, 139-144.	1.5	4
3571	Structures and stabilities of Au ⁺ Ar _n (n=1-6) clusters. <i>Computational and Theoretical Chemistry</i> , 2009, 899, 111-116.	1.5	15
3572	Structures, vibrational frequencies, and electron affinities of SF ₅ O _n /SF ₅ O _n ⁻ (n=1-3). <i>Computational and Theoretical Chemistry</i> , 2009, 900, 77-83.	1.5	4
3573	TD-DFT benchmark for indigo dyes. <i>Computational and Theoretical Chemistry</i> , 2009, 914, 100-105.	1.5	37
3574	Effect of electron-withdrawing group on the [3,3]-sigmatropic rearrangements of 1,5-enynes, 1,5-diyne and 1,2-diene-5-yne: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2009, 904, 69-73.	1.5	8
3575	From linear quaterthiophene to sulflower: A comparative theoretical study. <i>Computational and Theoretical Chemistry</i> , 2009, 912, 27-31.	1.5	11
3576	Quantitative estimates of transferability of the QTAIM descriptors. Case study of the substituted hydroxypyrimidines. <i>Computational and Theoretical Chemistry</i> , 2009, 906, 11-24.	1.5	24
3577	Molecular DFT structure and packing effect of thiodipropionic and dithiodiglycolic acids and salts. <i>Computational and Theoretical Chemistry</i> , 2009, 911, 52-57.	1.5	0
3578	Theoretical investigation of the hydrogen abstraction from CF ₃ CH ₂ CF ₃ by OH radicals, F, and Cl atoms: A dual-level direct dynamics study. <i>Computational and Theoretical Chemistry</i> , 2009, 913, 107-116.	1.5	15
3579	Theoretical study of the structure of neutral, radical and anionic monoperoxo carbonic acid. <i>Computational and Theoretical Chemistry</i> , 2009, 913, 131-138.	1.5	5
3580	Computational study of adsorption, diffusion, and dissociation of precursor species on the GaN (0001) surface during GaN MOCVD. <i>Surface Science</i> , 2009, 603, L31-L34.	0.8	14
3581	Density functional study of ethylamine and allylamine on Si(100)-2x1 and Ge(100)-2x1 surfaces. <i>Surface Science</i> , 2009, 603, 1055-1069.	0.8	9
3582	The role of electronic properties to the mutagenic activity of 1,6- and 3,6-dinitrobenzo[a]pyrene isomers. <i>Journal of Hazardous Materials</i> , 2009, 161, 1338-1346.	6.5	18
3583	Reaction mechanism of the binuclear zinc enzyme glyoxalase II: A theoretical study. <i>Journal of Inorganic Biochemistry</i> , 2009, 103, 274-281.	1.5	41
3584	Redox properties of (1-(2-pyridylazo)-2-naphthol)copper(II) encapsulated in Y Zeolite. <i>Microporous and Mesoporous Materials</i> , 2009, 117, 297-303.	2.2	23

#	ARTICLE	IF	CITATIONS
3585	Theoretical studies of stereoselectivities in the direct organocatalytic Mannich reactions involving ketimine. <i>Journal of Molecular Catalysis A</i> , 2009, 303, 1-8.	4.8	11
3586	Band envelope study of vapour phase FTIR spectra of acetamide aided by DFT. <i>Journal of Molecular Structure</i> , 2009, 920, 327-331.	1.8	2
3587	A mechanistic study of the electron capture dissociation of oligonucleotides. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 213-226.	1.2	13
3588	An experimental and theoretical investigation into the hydrolysis of dichloro(ethylenediamine)platinum(II) via electrospray mass spectrometry and density functional theory. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 1015-1029.	1.2	4
3589	Host-guest hydrogen atom transfer induced by electron capture. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 639-651.	1.2	7
3590	Hybrid QM/MM simulation of the hydration phenomena of dipalmitoylphosphatidylcholine headgroup. <i>Journal of Colloid and Interface Science</i> , 2009, 329, 410-415.	5.0	20
3591	Ferrihydrite reactivity toward carbon dioxide. <i>Journal of Colloid and Interface Science</i> , 2009, 337, 492-500.	5.0	79
3592	Computational study on transamination of alkylamides with NH ₃ during metalorganic chemical vapor deposition of tantalum nitride. <i>Journal of Crystal Growth</i> , 2009, 311, 3587-3591.	0.7	5
3593	Theoretical studies on magnetic interactions between Cu(II) ions in salen nucleobases. <i>Polyhedron</i> , 2009, 28, 1945-1949.	1.0	12
3594	Synthesis and structure of ferrocenylmethylphosphines, their borane adducts, and some related derivatives. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 2279-2289.	0.8	27
3595	Synthesis, ring transformations, IR-, NMR and DFT study of heterocycles with two ferrocenyl units. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 3732-3741.	0.8	20
3596	Triplet excited state characters and photosensitization mechanisms of $\hat{1}\pm$ -terthienyl: A theoretical study. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2009, 94, 51-53.	1.7	9
3597	Acidâ€“base behavior of 3-aminoquinoline in its ground and excited states. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2009, 207, 254-259.	2.0	18
3598	Exploring the oxidative decompositions of methyl esters: Methyl butanoate and methyl pentanoate as model compounds for biodiesel. <i>Proceedings of the Combustion Institute</i> , 2009, 32, 263-270.	2.4	56
3599	FT-IR vibrational spectrum and DFT:B3LYP/6-31G and B3LYP/6-311G structure and vibrational analysis of glycinateâ€“guanidoacetate nickel (II) complex: [Ni(Gly)(Gaa)]. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 72, 182-189.	2.0	41
3600	Spin-forbidden transitions in flavone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 73, 1-5.	2.0	12
3601	A DFT study of the vibrational spectra of 1-, and 2-nitrotriphenylene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 74, 579-587.	2.0	12
3602	Prediction of molecular properties and molecular spectroscopy with density functional theory: From fundamental theory to exchange-coupling. <i>Coordination Chemistry Reviews</i> , 2009, 253, 526-563.	9.5	927

#	ARTICLE	IF	CITATIONS
3603	The molecular and electronic structure of carbon-hydrogen bond activation and transition metal assisted hydrogen transfer. <i>Coordination Chemistry Reviews</i> , 2009, 253, 1202-1218.	9.5	76
3604	Spectroscopically validated density functional theory studies of the B12 cofactors and their interactions with enzyme active sites. <i>Coordination Chemistry Reviews</i> , 2009, 253, 779-794.	9.5	34
3605	Efficient, approximate and parallel Hartree-Fock and hybrid DFT calculations. A chain-of-spheres algorithm for the Hartree-Fock exchange. <i>Chemical Physics</i> , 2009, 356, 98-109.	0.9	2,010
3606	Atomic radical-molecule reaction N(4S)+NO ₂ (2A ₁): Mechanistic study. <i>Chemical Physics</i> , 2009, 358, 80-84.	0.9	3
3607	Ab initio molecular simulations with numeric atom-centered orbitals. <i>Computer Physics Communications</i> , 2009, 180, 2175-2196.	3.0	2,170
3608	Theoretical studies on the bonding of Cd ²⁺ to adenine and thymine: Tautomeric equilibrium and metalation in base pairing. <i>Chemical Physics Letters</i> , 2009, 467, 387-392.	1.2	13
3609	Theoretical study on the excited states and photodissociation mechanism of dimethyldisulfide. <i>Chemical Physics Letters</i> , 2009, 469, 242-246.	1.2	18
3610	Relation between bond order and delocalization index of QTAIM. <i>Chemical Physics Letters</i> , 2009, 468, 129-133.	1.2	105
3611	Theoretical studies on the reaction mechanism of O(1D) with CH ₃ OCF ₃ . <i>Chemical Physics Letters</i> , 2009, 471, 202-209.	1.2	1
3612	Mechanisms for H ₂ and CH ₃ elimination in the gas phase reaction of propyne with Zr: A DFT study. <i>Chemical Physics Letters</i> , 2009, 475, 34-39.	1.2	5
3613	Accurate multi-coefficient electronic structure methods MLSE(Cn)-DFT for thermochemical kinetics. <i>Chemical Physics Letters</i> , 2009, 475, 141-145.	1.2	3
3614	O-atom transfer reaction from N ₂ O to CO: A theoretical investigation. <i>Chemical Physics Letters</i> , 2009, 475, 202-207.	1.2	12
3615	Electron density distribution in cladribine (2-chloro-2-deoxyadenosine) - A drug against leukemia and multiple sclerosis - Studied by multinuclear NQR spectroscopy and DFT calculations. <i>Chemical Physics Letters</i> , 2009, 476, 293-302.	1.2	11
3616	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. <i>Chemical Physics Letters</i> , 2009, 478, 283-286.	1.2	9
3617	On the experimental structure of monoperoxocarbonic acid and the enthalpy of formation of carbonic acid, peroxyformic acid and monoperoxocarbonic acid in gas phase. <i>Chemical Physics Letters</i> , 2009, 480, 52-56.	1.2	3
3618	A theoretical study of the kinetics of OH radical addition to halogen substituted propenes. <i>Chemical Physics Letters</i> , 2009, 481, 29-33.	1.2	14
3619	Probing the 5f electrons in Am-I by hybrid density functional theory. <i>Chemical Physics Letters</i> , 2009, 482, 223-227.	1.2	10
3620	Stabilities of 3d transition-metal doped Si ₁₄ clusters. <i>Chemical Physics Letters</i> , 2009, 483, 30-34.	1.2	38

#	ARTICLE	IF	CITATIONS
3621	Synthesis and properties of conjugated thiophenes fused onto a dehydro[15]annulene scaffold. <i>Comptes Rendus Chimie</i> , 2009, 12, 385-394.	0.2	9
3622	Titanium complexes with \hat{I}^2 -ketoiminate chelate ligands for ethylene polymerization: The significant influence of substituents on structures and catalytic activities. <i>Inorganic Chemistry Communication</i> , 2009, 12, 796-799.	1.8	26
3623	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 395502.	0.7	18,183
3624	Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2420-2435.	2.3	942
3625	A Theoretical Study of Polyoxometalates and Dendrzyme Model Compounds. , 2009, , 129-142.		1
3626	GGA+U study of the incorporation of iodine in uranium dioxide. <i>European Physical Journal B</i> , 2009, 69, 203-209.	0.6	61
3627	Silver cluster induced absorption enhancement and conformation control of peptides. <i>European Physical Journal D</i> , 2009, 52, 203-206.	0.6	6
3628	Quantum mechanical and molecular mechanical simulation approaches bridging length and time scales for simulation of interface reactions in realistic environments. <i>European Physical Journal: Special Topics</i> , 2009, 177, 59-81.	1.2	3
3629	Growth of chiral single-walled carbon nanotube caps in the presence of a cobalt cluster. <i>Nanotechnology</i> , 2009, 20, 215601.	1.3	18
3630	“Mindless” DFT Benchmarking. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 993-1003.	2.3	215
3631	Performance of DFT Methods in the Calculation of Optical Spectra of TCF-Chromophores. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2835-2846.	2.3	54
3632	Tetramethylammonium benzporphodimethene and Isomeric \hat{I}^{\pm, \hat{I}^2} Unsaturated \hat{I}^3 Lactam Embedded N-Confused Tetramethylammonium benzporphodimethenes. <i>Chemistry - an Asian Journal</i> , 2009, 4, 164-173.	1.7	26
3633	“Half” Bonds in an Unusual Coordinated $S_{4 \times 2}$ Rectangle. <i>Chemistry - an Asian Journal</i> , 2009, 4, 302-313.	1.7	10
3634	The empirical valence bond as an effective strategy for computer-aided enzyme design. <i>Biotechnology Journal</i> , 2009, 4, 495-500.	1.8	11
3635	Computation of accurate excitation energies for large organic molecules with double-hybrid density functionals. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4611.	1.3	252
3636	Ion-Molecule Reactions of O^+ , S^+ -Dimethyl Methylphosphonothioate: Evidence for Intramolecular Sulfur Oxidation during VX Perhydrolysis. <i>Journal of Organic Chemistry</i> , 2009, 74, 9319-9327.	1.7	24
3637	Protonation of guanine quartets and quartet stacks: insights from DFT studies. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 278-287.	1.3	7
3638	Molecular Mechanism of the Z/E-Photoisomerization of Hemithioindigo Hemistilbene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11882-11887.	1.1	31

#	ARTICLE	IF	CITATIONS
3639	Diels-Alder Exo Selectivity in Terminal-Substituted Dienes and Dienophiles: Experimental Discoveries and Computational Explanations. <i>Journal of the American Chemical Society</i> , 2009, 131, 1947-1957.	6.6	103
3640	Theoretical study of solvent effect on one- and two-photon absorption properties of starburst DCM derivatives. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11538.	1.3	19
3641	Enhanced Efficiency of Organic Dye-Sensitized Solar Cells: Triphenylamine Derivatives. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16821-16833.	1.5	328
3642	Empirical and ab initio computation of the thermochemical parameters of amino acids: I. Monoamino carbonic acids and monoamino dicarbonic acids and their amides. <i>Russian Journal of General Chemistry</i> , 2009, 79, 453-457.	0.3	2
3643	On the possibility of template synthesis in the ternary system of vanadium(IV)-dithiooxamide-formaldehyde. <i>Russian Journal of General Chemistry</i> , 2009, 79, 1122-1128.	0.3	13
3644	Cage-like amines in the synthesis and oxidation of camphor-10-sulfonic acid amides. <i>Russian Journal of Organic Chemistry</i> , 2009, 45, 1007-1017.	0.3	12
3645	Carbon nanocontainers for gas storage. <i>Nanotechnologies in Russia</i> , 2009, 4, 806-815.	0.7	2
3646	Quantum chemical modeling of the adsorption of chloride ion and water molecule on group 1B metals. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2009, 45, 137-146.	0.3	6
3647	Quantum chemical modeling of hydroxide ion adsorption on group 1B metals from aqueous solutions. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2009, 45, 391-397.	0.3	7
3648	DFT B3LYP calculation of the spatial structure of Co(II), Ni(II), and Cu(II) template complexes formed in ternary systems metal(II) ion-dithiooxamide-formaldehyde. <i>Russian Journal of Inorganic Chemistry</i> , 2009, 54, 1952-1956.	0.3	46
3649	The thermodynamic characteristics of formation of organic molecule complexes with the magnesium ion in water: The results of quantum-chemical modeling. <i>Russian Journal of Physical Chemistry A</i> , 2009, 83, 565-574.	0.1	1
3650	Hydrogen-Bonding Interactions of (CF ₃) ₃ CH and (CF ₃) ₃ C ⁺ in the Gas Phase. An Experimental (FT-ICR) and Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6422-6429.	1.1	5
3651	Electronic Zero-Point Oscillations in the Strong-Interaction Limit of Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 743-753.	2.3	79
3652	Time-Dependent Density Functional Theory Study of the Electronic Excitation Spectra of Chlorophyllide a and Pheophorbide a in Solvents. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4817-4825.	1.2	29
3653	Kinetics of the Hydrogen Abstraction C ₂ H ₃ [•] + Alkane → C ₂ H ₄ + Alkyl Radical Reaction Class. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8327-8336.	1.1	20
3654	Protonation of the Side Group in Î ² - and Î ³ -Aminated Proline Analogues: Effects on the Conformational Preferences. <i>Journal of Organic Chemistry</i> , 2009, 74, 3101-3108.	1.7	9
3655	Germylene Energetics: Electron Affinities and Singlet-Triplet Gaps of GeX ₂ and GeXY Species (X, Y = H, CH ₃ , SiH ₃ , GeH ₃ , F, Cl, Br, I). <i>Journal of Physical Chemistry A</i> , 2009, 113, 8080-8090.	1.1	20
3656	Derivatives of Spiropentadiene Dication: New Species with Planar Tetracoordinate Carbon (ptC) atom. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3171-3176.	1.1	8

#	ARTICLE	IF	CITATIONS
3675	Catalytic and Thermal 1,2-Rearrangement of (±-Mercaptobenzyl)trimethylsilane. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11007-11014.	1.1	2
3676	QM/MM Study of the Monomeric Red Fluorescent Protein DsRed.M1. <i>Journal of Physical Chemistry B</i> , 2009, 113, 16622-16631.	1.2	21
3677	Effects of Doping on Electronic Structure and Correlations in Carbon Peapods. <i>ACS Nano</i> , 2009, 3, 1069-1076.	7.3	17
3678	Ab Initio Study of the Geometry, Stability, and Aromaticity of the Cyclic S ₂ N ₃ ⁺ Cation Isomers and Their Isoelectronic Analogues. <i>Inorganic Chemistry</i> , 2009, 48, 6773-6780.	1.9	15
3679	DFT Study on the Mechanism of Escherichia coli Inorganic Pyrophosphatase. <i>Journal of Physical Chemistry B</i> , 2009, 113, 6505-6510.	1.2	29
3680	Reactions of Aromatic Bifunctional Molecules on Silicon Surfaces: Nitrosobenzene and Nitrobenzene. <i>Journal of Physical Chemistry C</i> , 2009, 113, 6643-6653.	1.5	33
3681	Integrated Continuum Dielectric Approaches To Treat Molecular Polarizability and the Condensed Phase: Refractive Index and Implicit Solvation. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1785-1802.	2.3	18
3682	High-Resolution and Dispersed Fluorescence Examination of Vibronic Bands of Tryptamine: Spectroscopic Signatures for <i>L</i> _a / <i>L</i> _b Mixing near a Conical Intersection. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2456-2466.	1.1	28
3683	Helical Dendronized Polymers with Chiral Second-Generation Dendrons: Atomistic View and Driving Forces for Structure Formation. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14868-14876.	1.2	12
3684	Polarizability and Spin Density Correlate with the Relative Anaerobic Biodegradability of Alkylaromatic Hydrocarbons. <i>Environmental Science & Technology</i> , 2009, 43, 4995-5000.	4.6	6
3685	Using the ONIOM hybrid method to apply equation of motion CCSD to larger systems: Benchmarking and comparison with time-dependent density functional theory, configuration interaction singles, and time-dependent Hartree-Fock. <i>Journal of Chemical Physics</i> , 2009, 131, 134105.	1.2	15
3686	Mechanism of the Ni(O)-Catalyzed Vinylcyclopropane→Cyclopentene Rearrangement. <i>Journal of Organic Chemistry</i> , 2009, 74, 7822-7833.	1.7	59
3687	Electron Super-Rich Radicals. III. On the Peculiar Behavior of the Aminodihydroxymethyl Radical in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5855-5864.	1.1	5
3688	Ab Initio Investigation of Dissolution Mechanisms in Aluminosilicate Minerals. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1343-1352.	1.1	55
3689	To Flip or Not To Flip? Assessing the Inversion Barrier of the Tetraphenylene Framework with Enantiopure 2,15-Dideuteriotetraphenylene and 2,7-Dimethyltetraphenylene. <i>Journal of Organic Chemistry</i> , 2009, 74, 359-369.	1.7	56
3690	Gas-Phase Infrared Spectra of Vinyl Selenol and Vinyl Tellurol. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12857-12863.	1.1	7
3691	Block-Localized Density Functional Theory (BLDFT), Diabatic Coupling, and Their Use in Valence Bond Theory for Representing Reactive Potential Energy Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2702-2716.	2.3	110
3692	Kinetics of 1,4-Hydrogen Migration in the Alkyl Radical Reaction Class. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1564-1573.	1.1	39

#	ARTICLE	IF	CITATIONS
3693	Conformational Changes of meso-Aryl Substituted Expanded Porphyrins upon Protonation: Effects on Photophysical Properties and Aromaticity. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5794-5802.	1.2	33
3694	Protein Influence on Electronic Spectra Modeled by Multipoles and Polarizabilities. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 649-658.	2.3	67
3695	Gas-Phase Thermochemical Properties of the Damaged Base O6-Methylguanine versus Adenine and Guanine. <i>Journal of Organic Chemistry</i> , 2009, 74, 7429-7440.	1.7	44
3696	Theoretical Study of Adsorption of Group IIIA Nitrides on Si(111). <i>Journal of Physical Chemistry C</i> , 2009, 113, 5563-5567.	1.5	6
3697	<i>Ab initio</i> depolarization in self-assembled molecular monolayers: Beyond conventional density-functional theory. <i>Physical Review B</i> , 2009, 80, .	1.1	24
3698	Mechanisms for Formation of Diazocinones, Pyridazines, and Pyrazolines from Tetrazines: Oxyanion-Accelerated Pericyclic Cascades?. <i>Journal of Organic Chemistry</i> , 2009, 74, 4804-4811.	1.7	18
3699	Isolation, Biomimetic Synthesis, and Cytotoxic Activity of Bis(pseudopterane) Amines. <i>Journal of Natural Products</i> , 2009, 72, 1331-1334.	1.5	14
3700	Molecular Design toward High Hole Mobility Organic Semiconductors: Tetraceno[2,3-c]thiophene Derivatives of Ultrasmall Reorganization Energies. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16303-16306.	1.5	26
3701	Asymmetric Allylboration Reactions with Soderquist's Chiral 10-Substituted-9-borabicyclo[3.3.2]decanes: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2009, 74, 3562-3565.	1.7	9
3702	Discovering the Complex Chemistry of a Simple NiII/H3L System: Magnetostructural Characterization and DFT Calculations of Di- and Polynuclear Nickel(II) Compounds. <i>Inorganic Chemistry</i> , 2009, 48, 9861-9873.	1.9	29
3703	Photoarylation/Alkylation of Bromonaphthols. <i>Journal of Organic Chemistry</i> , 2009, 74, 1034-1041.	1.7	18
3704	Dependence of Response Functions and Orbital Functionals on Occupation Numbers. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 693-698.	2.3	3
3705	Stereoselective Control of Planar \pm -Dimethylsulfonium Benzyl Carbanions. Synthesis of Optically Pure <i>trans</i> -Aziridines. <i>Journal of Organic Chemistry</i> , 2009, 74, 4217-4224.	1.7	21
3706	Theoretical Study of Adsorption and Diffusion of Group IIIA Metals on Si(111). <i>Journal of Physical Chemistry C</i> , 2009, 113, 13924-13932.	1.5	14
3707	Controlled Isomerization of a Light-Driven Molecular Motor: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 3574-3580.	1.5	25
3708	Toward the Reactivity Prediction: Outersphere Electroreduction of Transition-Metal Ammine Complexes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 2881-2890.	1.5	8
3709	Kinetics of the Gas-Phase Reaction of OH with Chlorobenzene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10452-10459.	1.1	13
3710	Infrared Absorption Detection of Metal Ion-Deoxyguanosine Monophosphate Binding: Experimental and Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 283-291.	1.2	35

#	ARTICLE	IF	CITATIONS
3711	Intersystem Crossing and Characterization of Dark States in the Pyrimidine Nucleobases Uracil, Thymine, and 1-Methylthymine. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11809-11816.	1.1	104
3712	Insights into photodissociation dynamics of acetaldehyde from ab initio calculations and molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2009, 131, 054306.	1.2	34
3713	A General Boundary Potential for Hybrid QM/MM Simulations of Solvated Biomolecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3114-3128.	2.3	48
3714	Imino-oxy Acetic Acid Dealkylation as Evidence for an Inner-Sphere Alcohol Intermediate in the Reaction Catalyzed by Peptidylglycine β -Hydroxylating Monooxygenase. <i>Journal of the American Chemical Society</i> , 2009, 131, 10308-10319.	6.6	12
3715	Ab Initio Classical Trajectory Study of the Dissociation of Neutral and Positively Charged Methanimine (CH_2NH^+). <i>Journal of Physical Chemistry A</i> , 2009, 113, 9958-9964.	1.1	22
3716	Serendipitous Discovery of a Simple Compound with an Unsupported Ir-Ir Bond. <i>Organometallics</i> , 2009, 28, 1575-1578.	1.1	15
3717	Structure, Bonding, and Relative Stability of the Ground and Low-Lying Electronic States of CuO_2 . The Role of Exact Exchange. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1308-1317.	1.1	19
3718	Structural Evolution, Sequential Oxidation, and Chemical Bonding in Tritantalum Oxide Clusters: $\text{Ta}_3\text{O}_n^{+}$ and Ta_3O_n ($n = 1-8$). <i>Journal of Physical Chemistry A</i> , 2009, 113, 9804-9813.	1.1	48
3719	Molecular Dynamics Simulations of the Chromophore Binding Site of <i>Deinococcus radiodurans</i> Bacteriophytochrome Using New Force Field Parameters for the Phytychromobilin Chromophore. <i>Journal of Physical Chemistry B</i> , 2009, 113, 945-958.	1.2	26
3720	How a Single-Point Mutation in Horseradish Peroxidase Markedly Enhances Enantioselectivity. <i>Journal of the American Chemical Society</i> , 2009, 131, 11155-11160.	6.6	7
3721	Heterogeneous CO_2 Evolution from Oxidation of Aromatic Carbon-Based Materials. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8415-8420.	1.1	34
3722	Long-Range-Corrected Hybrids Based on a New Model Exchange Hole. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 754-762.	2.3	72
3723	Carboxyl-Catalyzed Prototropic Rearrangements in Histidine Peptide Radicals upon Electron Transfer: Effects of Peptide Sequence and Conformation. <i>Journal of the American Chemical Society</i> , 2009, 131, 16472-16487.	6.6	26
3724	Structural and Electronic Properties of Poly(thiaheterohelicene)s. <i>Journal of Physical Chemistry B</i> , 2009, 113, 15196-15203.	1.2	15
3725	Theoretical Analysis of Kinetic Isotope Effects on Proton Transfer Reactions between Substituted β -Methoxystyrenes and Substituted Acetic Acids. <i>Journal of the American Chemical Society</i> , 2009, 131, 13963-13971.	6.6	30
3726	Aromaticity of β -Oligothiophenes and Equivalent Oligothienoacenes. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1767-1775.	2.3	6
3727	Coordination of (Glycyl)glycine ($\text{C}_2\text{H}_5\text{NO}_2$) to Co^{2+} and Co^{3+} . <i>Journal of Physical Chemistry A</i> , 2009, 113, 8883-8892.	1.1	9
3728	Evidence of Disruption of Conjugation Involving Delta Bonds in Intramolecular Electronic Coupling. <i>Inorganic Chemistry</i> , 2009, 48, 11847-11852.	1.9	8

#	ARTICLE	IF	CITATIONS
3729	Effect of Stacking Interactions on the Spectra of the Monomer of PFBT: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10224-10230.	1.1	7
3730	Coordination Chemistry of Cyclohexane-1,2,4,5-tetracarboxylate (H_{4L}). Synthesis, Structure, and Magnetic Properties of Metal-Organic Frameworks with Conformation-Flexible H_{4L} Ligand. <i>Crystal Growth and Design</i> , 2009, 9, 2442-2450.	1.4	37
3731	Obtaining correct orbital ground states in f -electron systems using a nonspherical self-interaction-corrected LDA. <i>Physical Review B</i> , 2009, 80, .	1.1	37
3732	Theoretical Studies of N_2 Reduction to Ammonia in $Fe(dmpe)_2N_2$. <i>Inorganic Chemistry</i> , 2009, 48, 861-871.	1.9	43
3733	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5786-5799.	1.1	114
3734	Reactivities of Fe(IV) Complexes with Oxo, Hydroxo, and Alkylperoxo Ligands: An Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2009, 48, 11038-11047.	1.9	53
3735	First Energy Transfer and Davydov Splittings in Time-Dependent Density Functional Theory: Lessons from 2-Pyridone Dimer. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 873-880.	2.3	32
3736	Sensing Mechanism of Calix[4]arene-Substituted Poly(thiophene) Ion Receptor: Effects of the Selectivity on the Molecular Rigidity. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8284-8287.	1.2	4
3737	Probing Ligand Effects on the Redox Energies of $[4Fe^{\text{IV}}S]$ Clusters Using Broken-Symmetry Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5671-5676.	1.1	11
3738	Reductive Half-Reaction of Aldehyde Oxidoreductase toward Acetaldehyde: A Combined QM/MM Study. <i>Journal of the American Chemical Society</i> , 2009, 131, 4628-4640.	6.6	38
3739	Ab Initio Molecular Dynamics Simulations of the Infrared Spectra of $H_3O_2^+$ and $D_3O_2^+$. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1328-1336.	2.3	22
3740	Reactivity of $C_2H_5^+$ with Benzene: Formation of Ethylbenzenium Ions and Implications for Titanianospheric Chemistry. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11153-11160.	1.1	14
3741	Copper Corroles Are Inherently Saddled. <i>Inorganic Chemistry</i> , 2009, 48, 7794-7799.	1.9	103
3742	Density Functional Characterization of Adsorption and Decomposition of 1-Propanethiol on the Ga-Rich GaAs (001) Surface. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5685-5690.	1.1	8
3743	Conformational Preferences of 1-Amino-2-phenylcyclohexanecarboxylic Acid, a Phenylalanine Cyclohexane Analogue. <i>Journal of Organic Chemistry</i> , 2009, 74, 7834-7843.	1.7	7
3744	What Kinds of Ferryl Species Exist for Compound II of Chloroperoxidase? A Dialog of Theory with Experiment. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7912-7917.	1.2	28
3745	Extension to Negative Values of the Coupling Constant of Adiabatic Connection for Interaction-Strength Interpolation. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 708-711.	2.3	13
3746	Density Functional Theory Study of the Manganese-Containing Ribonucleotide Reductase from <i>Chlamydia trachomatis</i> : Why Manganese Is Needed in the Active Complex. <i>Biochemistry</i> , 2009, 48, 1878-1887.	1.2	41

#	ARTICLE	IF	CITATIONS
3747	Theoretical Studies on Structures and Spectroscopic Properties of Self-Assembled Bis(2,4,8,10-tetramethyl-9-methoxycarbonyl ethyldipyrin-3-yl)methane with Co(II). Journal of Physical Chemistry A, 2009, 113, 3375-3381.	1.1	14
3748	Catalytic Mechanism of Diaminopimelate Epimerase: A QM/MM Investigation. Journal of Chemical Theory and Computation, 2009, 5, 1915-1930.	2.3	17
3749	<i>ortho</i> -Substituted (Aryl)(3-nitrobenzo[<i>b</i>]thiophen-2-yl)amines: Study of the Electrochemical Behavior. Journal of Physical Chemistry A, 2009, 113, 10260-10263.	1.1	3
3750	Ab initio Study of the Structural, Tautomeric, Pairing, and Electronic Properties of Seleno-Derivatives of Thymine. Journal of Physical Chemistry B, 2009, 113, 14465-14472.	1.2	15
3751	Effect of Metal Cluster-Cap Interactions on the Catalyzed Growth of Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2009, 113, 698-709.	1.5	32
3752	Molecular Actuators Designed with S ^N (sp ²) Hemibonds Attached to a Conformationally Flexible Pivot. Chemistry of Materials, 2009, 21, 2149-2157.	3.2	4
3753	Mechanistic Study of the sPLA ₂ -Mediated Hydrolysis of a Thio-ester Pro Anticancer Ether Lipid. Journal of the American Chemical Society, 2009, 131, 12193-12200.	6.6	57
3754	Hybrid density functional calculations of the band gap of $Ga_{1-x}Mn_x$. Physical Review B, 2009, 80, .	1.1	41
3755	First Half-Reaction Mechanism of Nitric Oxide Synthase: The Role of Proton and Oxygen Coupled Electron Transfer in the Reaction by Quantum Mechanics/Molecular Mechanics. Journal of Physical Chemistry B, 2009, 113, 336-346.	1.2	40
3756	Negative differential resistance in fused thiophene trimer. Computational Materials Science, 2009, 45, 889-898.	1.4	22
3757	Ab initio calculations of Fe-Ni clusters. Computational Materials Science, 2009, 46, 367-375.	1.4	22
3758	Photophysical and charge-transport properties of hole-blocking material-TAZ: A theoretical study. Synthetic Metals, 2009, 159, 1767-1771.	2.1	6
3759	Highly fluorescent oligomers with donor and acceptor groups: DFT calculations and experiments. Synthetic Metals, 2009, 159, 2211-2214.	2.1	3
3760	Altered Activity and Physicochemical Properties of Short Cationic Antimicrobial Peptides by Incorporation of Arginine Analogues. Molecular Pharmaceutics, 2009, 6, 996-1005.	2.3	45
3761	Prediction of the Intrinsic Hydrogen Bond Acceptor Strength of Organic Compounds by Local Molecular Parameters. Journal of Chemical Information and Modeling, 2009, 49, 956-962.	2.5	43
3762	Is Cerocene Really a Ce(III) Compound? All-Electron Spin-Orbit Coupled CASPT2 Calculations on $M(\bar{f})_{8-C_{8}H_{8}}_{2}$ (M = Th, Pa, Ce). Journal of Physical Chemistry A, 2009, 113, 2896-2905.	1.1	72
3763	Modeling an Electronic Conductor Based on Natural Peptide Sequences. Biomacromolecules, 2009, 10, 2338-2343.	2.6	11
3764	DFT Study on Bifunctional Chiral Brønsted Acid-Catalyzed Asymmetric Hydrophosphonylation of Imines. Journal of Organic Chemistry, 2009, 74, 3266-3271.	1.7	82

#	ARTICLE	IF	CITATIONS
3765	The calculation of adiabatic-connection curves from full configuration-interaction densities: Two-electron systems. <i>Journal of Chemical Physics</i> , 2009, 130, 104111.	1.2	64
3766	Switchable Molecular Conductivity. <i>Journal of the American Chemical Society</i> , 2009, 131, 10447-10451.	6.6	23
3767	Interrelations between the Mesomeric and Electronegativity Effects in <i>Para</i> -Substituted Derivatives of Phenol/Phenolate and Aniline/Anilide H-Bonded Complexes: A DFT-Based Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5800-5805.	1.1	5
3770	Modeling Properties and Reactivity of Quinone Methides by DFT Calculations. , 0, , 33-67.		2
3771	The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 808-821.	2.3	462
3772	Consequences of Conformational Preorganization in Sesquiterpene Biosynthesis: Theoretical Studies on the Formation of the Bisabolene, Curcumene, Acoradiene, Zizaene, Cedrene, Duprezianene, and Sesquithuriferol Sesquiterpenes. <i>Journal of the American Chemical Society</i> , 2009, 131, 7999-8015.	6.6	113
3773	Molecular acidity: A quantitative conceptual density functional theory description. <i>Journal of Chemical Physics</i> , 2009, 131, 164107.	1.2	58
3774	First principles computational materials design for energy storage materials in lithium ion batteries. <i>Energy and Environmental Science</i> , 2009, 2, 589.	15.6	456
3775	Plicatin B conformational landscape and affinity to copper (I and II) metal cations. A DFT study. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 776-790.	1.3	51
3777	Hybrid density-functional calculation of the electronic and magnetic structures of tetragonal CuO. <i>Physical Review B</i> , 2009, 80, .	1.1	27
3778	Unraveling the Jahn-Teller effect in Mn-doped GaN using the Heyd-Scuseria-Ernzerhof hybrid functional. <i>Physical Review B</i> , 2009, 79, .	1.1	122
3779	Polaronic Hole Trapping in Doped BaBiO_3 . <i>Physical Review Letters</i> , 2009, 102, 256402.	2.9	93
3780	Doubly $\hat{\text{I}}^2$ -Functionalized Meso-Meso Directly Linked Porphyrin Dimer Sensitizers for Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2009, 113, 21956-21963.	1.5	78
3782	Efficient and accurate approximations to the local coupled cluster singles doubles method using a truncated pair natural orbital basis. <i>Journal of Chemical Physics</i> , 2009, 131, 064103.	1.2	468
3783	Periodic DFT modeling of bulk and surface properties of MgCl_2 . <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6525.	1.3	54
3784	A DFT Study of Nucleobase Dealkylation by the DNA Repair Enzyme AlkB. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4887-4898.	1.2	64
3785	Adsorption of Methimazole on Silver Nanoparticles: FTIR, Raman, and Surface-Enhanced Raman Scattering Study Aided by Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2009, 113, 7091-7100.	1.5	71
3786	The lithiation and acyl transfer reactions of phosphine oxides, sulfides and boranes in the synthesis of cyclopropanes. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 1329.	1.5	11

#	ARTICLE	IF	CITATIONS
3787	Low-lying absorption and emission spectra of pyrene, 1,6-dithiaperylene, and tetrathiafulvalene: A comparison between ab initio and time-dependent density functional methods. <i>Journal of Chemical Physics</i> , 2009, 131, 224315.	1.2	32
3788	Spectral Properties of Spirooxazine Photochromes: TD-DFT Insights. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13004-13012.	1.1	34
3789	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. <i>Physical Review B</i> , 2009, 80, .	1.1	47
3790	Proton Transfer on the Molecular Surface of Proteins and Model Systems. <i>Israel Journal of Chemistry</i> , 2009, 49, 149-153.	1.0	5
3791	Density Functional Theory Study of the Adsorption of Au Atom on Cerium Oxide: Effect of Low-Coordinated Surface Sites. <i>Journal of Physical Chemistry C</i> , 2009, 113, 4948-4954.	1.5	54
3792	First Principles Effective Electronic Couplings for Hole Transfer in Natural and Size-Expanded DNA. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9402-9415.	1.2	64
3793	Rate Limiting Step Precedes C ^α -C Bond Formation in the Archetypical Proline-Catalyzed Intramolecular Aldol Reaction. <i>Journal of the American Chemical Society</i> , 2009, 131, 1632-1633.	6.6	63
3795	Utilizing the Charge Field Effect on Amide ¹⁵ N Chemical Shifts for Protein Structure Validation. <i>Journal of Physical Chemistry B</i> , 2009, 113, 347-358.	1.2	5
3798	Photophysics of phenalenone: quantum-mechanical investigation of singlet [→] triplet intersystem crossing. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1688.	1.3	31
3799	Probing the Electronic and Structural Properties of the Niobium Trimer Cluster and Its Mono- and Dioxides: Nb ₃ O _n (n = 1, 2) and Nb ₃ O _n (n = 0, 2). <i>Journal of Physical Chemistry A</i> , 2009, 113, 3866-3875.	1.1	55
3800	Unexpected Regioselectivity in the Synthesis of Pyranonaphthoquinone via the Diels-Alder Reaction. <i>Organic Letters</i> , 2009, 11, 4628-4631.	2.4	13
3801	Parallel multireference configuration interaction calculations on mini- β -carotenes and β -carotene. <i>Journal of Chemical Physics</i> , 2009, 130, 044708.	1.2	111
3802	DFT Calculations on Heterocyclacenes. <i>Organic Letters</i> , 2009, 11, 725-728.	2.4	22
3803	Accurate Calculation of Zero-Field Splittings of (Bio)inorganic Complexes: Application to an {FeNO} ⁷ (S = 3/2) Compound. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9150-9156.	1.1	22
3804	Synthesis, Spectroscopy, Crystal Structure, Electrochemistry, and Quantum Chemical and Molecular Dynamics Calculations of a 3-Anilino Difluoroboron Dipyrromethene Dye. <i>Journal of Physical Chemistry A</i> , 2009, 113, 439-447.	1.1	98
3805	Calculation of Electronic Circular Dichroism Spectra with Time-Dependent Double-Hybrid Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 767-776.	1.1	133
3807	NMR tensors in planar hydrocarbons of increasing size. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11404.	1.3	27
3808	Human Insulin-Degrading Enzyme Working Mechanism. <i>Journal of the American Chemical Society</i> , 2009, 131, 14804-14811.	6.6	56

#	ARTICLE	IF	CITATIONS
3809	Origin of Stereoselectivity in the Imidazolidinone-Catalyzed Reductions of Cyclic $\hat{1}\pm, \hat{1}2$ -Unsaturated Ketones. <i>Organic Letters</i> , 2009, 11, 4298-4301.	2.4	40
3810	Density Functional Theory Calculations of the Optical Rotation and Electronic Circular Dichroism: The Absolute Configuration of the Highly Flexible <i>trans</i> -Isocytosazine Revised. <i>Journal of Organic Chemistry</i> , 2009, 74, 8051-8063.	1.7	50
3811	QTAIM Study of an $\hat{1}\pm$ -Helix Hydrogen Bond Network. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10957-10964.	1.2	52
3812	Hydrogen-Bond-Assisted Epoxidation of Homoallylic and Allylic Alcohols with Hydrogen Peroxide Catalyzed by Selenium-Containing Dinuclear Peroxotungstate. <i>Journal of the American Chemical Society</i> , 2009, 131, 6997-7004.	6.6	98
3813	Absorption and fluorescence properties of oligothiophene biomarkers from long-range-corrected time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4498.	1.3	145
3814	Comparison of Global Reactivity Descriptors Calculated Using Various Density Functionals: A QSAR Perspective. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2744-2753.	2.3	142
3815	Large carrier mobilities in octathio[8]circulene crystals: a theoretical study. <i>Journal of Materials Chemistry</i> , 2009, 19, 4356.	6.7	51
3816	Assessment of Orbital-Optimized, Spin-Component Scaled Second-Order Many-Body Perturbation Theory for Thermochemistry and Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3060-3073.	2.3	199
3817	Kinetics of Enol Formation from Reaction of OH with Propene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3177-3185.	1.1	57
3818	Spin-Selective Charge Transport Pathways through <i>p</i> -Oligophenylene-Linked Donor-Bridge-Acceptor Molecules. <i>Journal of the American Chemical Society</i> , 2009, 131, 17655-17666.	6.6	83
3819	Examination of DFT and TDDFT Methods II. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10873-10879.	1.1	19
3820	Improvement of the ab initio embedded cluster method for luminescence properties of doped materials by taking into account impurity induced distortions: The example of $Y_{[2]}O_{[3]}:Bi_{[3+]}$. <i>Journal of Chemical Physics</i> , 2009, 131, 194501.	1.2	20
3821	Dioxygen and Water Activation Processes on Multi-Ru-Substituted Polyoxometalates: Comparison with the α -Blue-Dimer-Water Oxidation Catalyst. <i>Journal of the American Chemical Society</i> , 2009, 131, 6844-6854.	6.6	88
3822	DFT Study on the Mechanism and Regioselectivity of Gold(I)-Catalyzed Synthesis of Highly Substituted Furans Based on 1-(1-Alkynyl)cyclopropyl Ketones with Nucleophiles. <i>Organometallics</i> , 2009, 28, 741-748.	1.1	41
3823	Ab Initio Modeling of Proton Transfer in Phosphoric Acid Clusters. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9193-9201.	1.1	65
3824	Hydrogen Bonding and Stacking π - π Interactions in Solid 6-Thioguanine and 6-Mercaptopurine (Antileukemia and Antineoplastic Drugs) Studied by NMR-NQR Double Resonance Spectroscopy and Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8781-8790.	1.1	18
3825	Optical absorption and emission properties of rubrene: insight from a combined experimental and theoretical study. <i>New Journal of Physics</i> , 2009, 11, 015001.	1.2	105
3826	Synthesis and <i>C</i> -Alkylation of Hindered Aldehyde Enamines. <i>Journal of Organic Chemistry</i> , 2009, 74, 1019-1028.	1.7	38

#	ARTICLE	IF	CITATIONS
3827	Robust recognition of malonate and 2-amino-4-picolinium in conjunction with M(ii) as a triad (M =) Tj ETQqO O O rgBT /Overlock 10 Tf 50 Dalton Transactions, 2009, , 7617.	1.6	26
3828	Enhanced acidity of cyclopenta-2,4-dienylborane and its Al and Ga analogues. The role of aromatization. Physical Chemistry Chemical Physics, 2009, 11, 8759.	1.3	6
3829	Can short-range hybrids describe long-range-dependent properties?. Journal of Chemical Physics, 2009, 131, 044108.	1.2	426
3830	Screened hybrid density functionals for solid-state chemistry and physics. Physical Chemistry Chemical Physics, 2009, 11, 443-454.	1.3	384
3831	Effects of Substrate, Protein Environment, and Proximal Ligand Mutation on Compound I and Compound O of Chloroperoxidase. Journal of Physical Chemistry A, 2009, 113, 11763-11771.	1.1	26
3832	DFT studies on catalytic properties of isolated and carbon nanotube supported Pd ₉ cluster: adsorption, fragmentation and diffusion of hydrogen. Physical Chemistry Chemical Physics, 2009, 11, 4077.	1.3	34
3833	Assessment of the Accuracy of Theoretical Methods for Calculating ²⁷ Al Nuclear Magnetic Resonance Shielding Tensors of Aquated Aluminum Species. Journal of Physical Chemistry A, 2009, 113, 5138-5143.	1.1	21
3834	Explorations into Neolignan Biosynthesis: Concise Total Syntheses of Helicterin B, Helisorin, and Helisterculin A from a Common Intermediate. Journal of the American Chemical Society, 2009, 131, 1745-1752.	6.6	53
3835	Fluorine substituent effects on dihydrogen bonding of transition metal hydrides. Physical Chemistry Chemical Physics, 2009, 11, 7231.	1.3	10
3836	Assessing the Performance of Density Functional Theory for the Electronic Structure of Metal ^d -Salens: The d ⁶ -Metals. Journal of Physical Chemistry A, 2009, 113, 9231-9236.	1.1	30
3837	Localized Orbital Corrections for the Barrier Heights in Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 2996-3009.	2.3	21
3838	Modes of inactivation of trichodiene synthase by a cyclopropane-containing farnesyldiphosphate analog. Organic and Biomolecular Chemistry, 2009, 7, 4101.	1.5	26
3839	Experimental and theoretical studies of complexes of [PbmAg] ⁿ⁺ (m = 1-4). Physical Chemistry Chemical Physics, 2009, 11, 1043.	1.3	7
3840	On the Mechanism of the Palladium Catalyzed Intramolecular Pauson-Khand-Type Reaction. Journal of Organic Chemistry, 2009, 74, 5049-5058.	1.7	54
3841	Modulation of Tris(o-phenylenedioxy)cyclotrisphosphazene (TPP) Properties for Zeolite Use: Effect of π -Conjugation Length and CH/N Heterosubstitution. Journal of Physical Chemistry A, 2009, 113, 246-254.	1.1	2
3842	Atomization energies of the carbon clusters C _n (n = 2-10) revisited by means of W4 theory as well as density functional, G _n , and CBS methods. Molecular Physics, 2009, 107, 977-990.	0.8	41
3843	NMR shielding as a probe of intermolecular interactions: ab initio and density functional theory studies. Physical Chemistry Chemical Physics, 2009, 11, 10331.	1.3	37
3844	Spectroscopic signatures for planar equilibrium geometries in methyl-substituted oligothiophenes. Physical Chemistry Chemical Physics, 2009, 11, 984-990.	1.3	43

#	ARTICLE	IF	CITATIONS
3845	Revisiting the planarity of nucleic acid bases: Pyramidilization at glycosidic nitrogen in purine bases is modulated by orientation of glycosidic torsion. <i>Nucleic Acids Research</i> , 2009, 37, 7321-7331.	6.5	27
3847	A comprehensive investigation of the electronic spectral and photophysical properties of conjugated naphthalene-thiophene oligomers. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 8706.	1.3	30
3848	Spectroscopic properties of phenolic and quinoid carotenoids: a combined theoretical and experimental study. <i>Photochemical and Photobiological Sciences</i> , 2009, 8, 270-278.	1.6	18
3849	Short cut to 1,2,3-triazole-based p38 MAP kinase inhibitors via [3+2]-cycloaddition chemistry. <i>New Journal of Chemistry</i> , 2009, 33, 1010-1016.	1.4	32
3850	Intermediate spin ground state of an isosceles triangular [MnII ₃] complex. <i>Dalton Transactions</i> , 2009, , 8162.	1.6	6
3851	The effects of C by N replacement on the hydrogen bonding of malonaldehyde: N-formylformimidic acid, N-(hydroxymethyl)formamide and related compounds. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 762-769.	1.3	15
3852	Structure and internal rotation in the S ₀ and S ₁ states of o-toluidine studied by high resolution UV spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4311.	1.3	5
3853	A theoretical study on the hydrolysis process of two Keppler-type antitumor complexes [TzH][trans-RuCl ₄ (Tz) ₂] and [2-NH ₂ TzH][trans-RuCl ₄ (2-NH ₂ Tz) ₂]. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3401.	1.3	11
3854	Neutral and reduced Roussin's red salt ester [Fe ₂ ($\frac{1}{4}$ -RS) ₂ (NO) ₄] (R) Tj ETQq0 0 0 rgBT /Overloc spectroscopic, electrochemical and density functional theoretical investigations. <i>Dalton Transactions</i> , 2009, , 777-786.	1.6	48
3855	Quantum dynamics of light-driven chiral molecular motors. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1662.	1.3	19
3857	Development of a new analysis method evaluating adsorption energies for the respective ion-exchanged sites on alkali-metal ion-exchanged ZSM-5 utilizing CO as a probe molecule: IR-spectroscopic and calorimetric studies combined with a DFT method. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5041.	1.3	9
3858	Substituent effects on ⁶¹ Ni NMR chemical shifts. <i>Dalton Transactions</i> , 2009, , 6037.	1.6	11
3859	Hydrogenation of imines by phosphonium borate zwitterions: a theoretical study. <i>Dalton Transactions</i> , 2009, , 1321.	1.6	39
3860	Effect of ring fusion on the amplified spontaneous emission properties of oligothiophenes. <i>Journal of Materials Chemistry</i> , 2009, 19, 6556.	6.7	17
3861	Dynamics of guest molecules in PHTP inclusion compounds as probed by solid-state NMR and fluorescence spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4996.	1.3	17
3862	A comparative computational study of matrix-peptide interactions in MALDI mass spectrometry: the interaction of four tripeptides with the MALDI matrices 2,5-dihydroxybenzoic acid, β -cyano-4-hydroxy-cinnamic acid and 3,5-dihydroxybenzoic acid. <i>Molecular Physics</i> , 2009, 107, 777-788.	0.8	4
3863	Structures and electron affinities of BrO ₂ F ₂ and BrO ₂ F ₃ . <i>Molecular Physics</i> , 2009, 107, 701-709.	0.8	2
3864	Side-Chain to Backbone Interactions Dictate the Conformational Preferences of a Cyclopentane Arginine Analogue. <i>Journal of Organic Chemistry</i> , 2009, 74, 2403-2412.	1.7	7

#	ARTICLE	IF	CITATIONS
3865	<i>In Silico</i> Molecular Engineering for a Targeted Replacement in a Tumor-Homing Peptide. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7879-7889.	1.2	16
3866	Structure of the Alanine Hydration Shell as Probed by NMR Chemical Shifts and Indirect Spin-Spin Coupling. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14698-14707.	1.2	47
3867	A Density Functional Theory Study of the Magnetic Exchange Coupling in Dinuclear Manganese(II) Inverse Crown Structures. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14008-14013.	1.1	17
3868	Side Chain Flexibilities in the Human Ether-a-go-go Related Gene Potassium Channel (hERG) Together with Matched-Pair Binding Studies Suggest a New Binding Mode for Channel Blockers. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 4266-4276.	2.9	44
3869	CH ₂ Interaction in Benzene and Substituted Derivatives with Halomethane: A Combined Density Functional and Dispersion-Corrected Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10113-10118.	1.1	28
3870	Neighbouring group participation vs. addition to oxacarbenium ions: studies on the synthesis of mycobacterial oligosaccharides. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 4842.	1.5	51
3871	On the origin of the regioselectivity in glycosylation reactions of 1,2-diols. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 1471.	1.5	16
3872	Synergistic activation of the Diels-Alder reaction by an organic catalyst and substituents: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 1304.	1.5	18
3873	Localized and Itinerant States in Lanthanide Oxides United by $G < W < \%$ Physical Review Letters, 2009, 102, 126403.	2.9	156
3874	Electropolymerizable 2,2-Carboranyldithiophenes. Structure-Property Investigations of the Corresponding Conducting Polymer Films by Electrochemistry, UV-Visible Spectroscopy and Conducting Probe Atomic Force Microscopy. <i>Macromolecules</i> , 2009, 42, 2981-2987.	2.2	46
3875	A first-principles study of bulk oxide formation on Pd(100). <i>Journal of Chemical Physics</i> , 2009, 131, 054701.	1.2	53
3876	The chemistry of reactive radical intermediates in combustion and the atmosphere. <i>Advances in Physical Organic Chemistry</i> , 2009, , 79-134.	0.5	8
3877	Synthesis, crystal structures and nonlinear optical properties of three TCF-based chromophores. <i>CrystEngComm</i> , 2009, 11, 589-596.	1.3	17
3878	C ₇₀ Oxides and Ozonides and the Mechanism of Ozonolysis on the Fullerene Surface. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9891-9898.	1.1	19
3879	A Combined Theoretical and Experimental Study of the Ammonia Tunnel in Carbamoyl Phosphate Synthetase. <i>Journal of the American Chemical Society</i> , 2009, 131, 10211-10219.	6.6	30
3880	Molecular Oxygen Activation and Proton Transfer Mechanisms in Lanosterol 14 α -Demethylase Catalysis. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8170-8182.	1.2	29
3881	Histidine-Containing Radicals in the Gas Phase. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7347-7366.	1.2	25
3882	Experimental and Theoretical Investigation Into Hydrogen Storage via Spillover in IRMOF-8. <i>Journal of Physical Chemistry C</i> , 2009, 113, 3222-3231.	1.5	68

#	ARTICLE	IF	CITATIONS
3883	Theoretical Investigation of Square-Planar MXe_4^{2+} ($M = Cu, Ag, Au$) Cations. <i>Australian Journal of Chemistry</i> , 2009, 62, 1556.	0.5	2
3884	Chiral recognition in bicyclic guanidines. <i>Collection of Czechoslovak Chemical Communications</i> , 2009, 74, 299-312.	1.0	5
3885	A density functional theory study of the correlation between analyte basicity, ZnPc adsorption strength, and sensor response. <i>Journal of Chemical Physics</i> , 2009, 130, 204307.	1.2	20
3886	Electronic and optical properties of silole-based derivatives. <i>Pigment and Resin Technology</i> , 2009, 38, 387-391.	0.5	4
3887	Theoretical Study on the Mechanism of Low-Energy Dissociative Electron Attachment for Uracil. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4795-4801.	1.1	27
3888	Unexpected Gas-Phase Ion Chemistry Results Unraveled by Computational Chemistry. <i>Current Organic Chemistry</i> , 2010, 14, 1600-1611.	0.9	6
3889	Calculating charged defects using CRYSTAL. <i>Journal of Physics: Conference Series</i> , 2010, 242, 012004.	0.3	6
3895	On Occupied-orbital Dependent Exchange-correlation Functionals: From Local Hybrids to Becke's B05 Model. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 545-567.	1.4	8
3897	Application of Real-time Time-dependent Density Functional Theory with the CVB3LYP Functional to Core Excitations. <i>Chemistry Letters</i> , 2010, 39, 407-409.	0.7	19
3898	Quantitative Structure-Toxicity Prediction of $\log(1/EC_{50})$ for Some Benzene Derivatives from Their Density Functional Theory Calculated Molecular Descriptors. <i>Bulletin of the Chemical Society of Japan</i> , 2010, 83, 345-350.	2.0	5
3899	Structure of the template complex formed in the Co(III)-dithiooxamide-acetone ternary system during complex formation in the $KCoFe(CN)_6$ -gelatin immobilized matrices. <i>Russian Journal of Inorganic Chemistry</i> , 2010, 55, 1243-1247.	0.3	20
3900	Theoretical and experimental study on cyclic 6-methyl-2,3,4-tris(hydroxymethyl)pyridin-5-ol acetonides. <i>Russian Journal of Organic Chemistry</i> , 2010, 46, 561-567.	0.3	17
3901	A hybrid DFT description of the (0001) surface of americium-I. <i>European Physical Journal B</i> , 2010, 78, 13-22.	0.6	1
3902	Mechanism of Enantioselective $C\text{--}C$ Bond Formation with Bifunctional Chiral Ru Catalysts: NMR and DFT Study. <i>Journal of the American Chemical Society</i> , 2010, 132, 16637-16650.	6.6	37
3903	Electric-Field-Assisted Electron Transfer in a Porphine-Quinone Complex: A Theoretical Study. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 805-816.	2.3	13
3904	Systematic Theoretical Study of the Zero-Field Splitting in Coordination Complexes of Mn(III). Density Functional Theory versus Multireference Wave Function Approaches. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10750-10758.	1.1	129
3905	Computational Explorations of Mechanisms and Ligand-Directed Selectivities of Copper-Catalyzed Ullmann-Type Reactions. <i>Journal of the American Chemical Society</i> , 2010, 132, 6205-6213.	6.6	324
3906	Chemistry of Vinylidenecyclopropanes. <i>Chemical Reviews</i> , 2010, 110, 5883-5913.	23.0	177

#	ARTICLE	IF	CITATIONS
3907	Redox Multifunctionality in a Series of Pt ^{II} Dithiolene Complexes of a Tetrathiafulvalene-Based Diphosphine Ligand. <i>Chemistry - an Asian Journal</i> , 2010, 5, 169-176.	1.7	23
3908	The Origin of the Halogen Effect on the Phthalocyanine Green Pigments. <i>Chemistry - an Asian Journal</i> , 2010, 5, 1341-1346.	1.7	4
3909	Reactions of H ₂ , CH ₄ , C ₂ H ₆ , and C ₃ H ₈ with [(MgO) _n] ⁺ Clusters Studied by Density Functional Theory. <i>ChemCatChem</i> , 2010, 2, 819-826.	1.8	51
3910	Mechanism of the Organocatalyzed Decarboxylative Knoevenagel-Doebner Reaction. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13086-13092.	1.1	15
3911	A Computational Investigation of Organic Dyes for Dye-Sensitized Solar Cells: Benchmark, Strategies, and Open Issues. <i>Journal of Physical Chemistry C</i> , 2010, 114, 7205-7212.	1.5	328
3912	Ab Initio Determination of Ground and Excited State Oxidation Potentials of Organic Chromophores for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22742-22750.	1.5	135
3913	Peroxo-Iron Mediated Deformylation in Sterol 14 α -Demethylase Catalysis. <i>Journal of the American Chemical Society</i> , 2010, 132, 10293-10305.	6.6	66
3914	Photoinduced Energy-Transfer and Electron-Transfer Processes in Dye-Sensitized Solar Cells: TDDFT Insights for Triphenylamine Dyes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16716-16725.	1.5	105
3915	Aggregation of Organic Dyes on TiO ₂ in Dye-Sensitized Solar Cells Models: An <i>ab Initio</i> Investigation. <i>ACS Nano</i> , 2010, 4, 556-562.	7.3	249
3916	Dependence of Excited State Potential Energy Surfaces on the Spatial Overlap of the Kohn-Sham Orbitals and the Amount of Nonlocal Hartree-Fock Exchange in Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2315-2324.	2.3	108
3917	Spin-flip time dependent density functional theory applied to excited states with single, double, or mixed electron excitation character. <i>Journal of Chemical Physics</i> , 2010, 133, 114104.	1.2	88
3918	Luminescent, Redox-Active Diphenothiazine Dumbbells Expanded by Conjugated Arenes and Heteroarenes. <i>Journal of Organic Chemistry</i> , 2010, 75, 8591-8603.	1.7	15
3919	Molecular structure and spectroscopic properties of polyaromatic heterocycles by first principle calculations: spectroscopic shifts with the adsorption of thiophene on phyllosilicate surface. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 83-95.	0.5	42
3920	Fluorene-based oligomers as red light-emitting materials: a density functional theory study. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 305-314.	0.5	3
3921	Theoretical investigation into charge mobility in 4,4'-bis(1-naphthylphenylamino)biphenyl. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 759-763.	0.5	18
3922	Overcoming systematic DFT errors for hydrocarbon reaction energies. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 429-442.	0.5	51
3923	DFT spin-orbit coupling between singlet and triplet excited states: A case of psoralen compounds. <i>Chemical Physics Letters</i> , 2010, 490, 90-96.	1.2	34
3924	DFT simulation of Mg/Al hydrotalcite with different intercalated anions: Periodic structure and solvating effects on the iodide/triiodide redox couple. <i>Chemical Physics Letters</i> , 2010, 494, 274-278.	1.2	14

#	ARTICLE	IF	CITATIONS
3925	Anchoring Pd nanoclusters onto pristine and functionalized single-wall carbon nanotubes: A combined DFT and experimental study. <i>Chemical Physics Letters</i> , 2010, 497, 103-107.	1.2	34
3926	Assignment of the He@C ₈₄ isomers in experimental NMR spectra using density functional calculations. <i>Chemical Physics Letters</i> , 2010, 500, 54-58.	1.2	15
3927	Unprecedented triphosphinine iron interactions: Intramolecular electron transfer, reactivity round a corner, and a low-activated ring element exchange reaction. <i>Comptes Rendus Chimie</i> , 2010, 13, 1203-1212.	0.2	14
3928	The bioisosteric similarity of the tetrazole and carboxylate anions: Clues from the topologies of the electrostatic potential and of the electron density. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 1868-1872.	2.6	65
3929	Î ² -Naphthoflavone analogs as potent and soluble aryl hydrocarbon receptor agonists: Improvement of solubility by disruption of molecular planarity. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 1194-1203.	1.4	39
3930	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. <i>Chemical Physics</i> , 2010, 375, 26-34.	0.9	124
3931	Improvement of the efficiency of thiophene-bridged compounds for dye-sensitized solar cells. <i>Chemical Physics</i> , 2010, 376, 56-68.	0.9	120
3932	Multi-walled carbon nanotubes as the gas chromatographic stationary phase: Role of their functionalization in the analysis of aliphatic alcohols and esters. <i>Journal of Chromatography A</i> , 2010, 1217, 7275-7281.	1.8	53
3933	Formation and sigmatropic rearrangement of PhCOC(NO ₂)CH ₂ cycloadducts of 1,3-cyclohexadiene: a theoretical study. <i>Tetrahedron</i> , 2010, 66, 845-851.	1.0	6
3934	Novel carbon-bridged citrinin dimers from a volcano ash-derived fungus <i>Penicillium citrinum</i> and their cytotoxic and cell cycle arrest activities. <i>Tetrahedron</i> , 2010, 66, 9286-9290.	1.0	28
3935	Atomic-scale determination of DNA conformational response to strained furanose: a static mode approach. <i>Tetrahedron</i> , 2010, 66, 9123-9128.	1.0	4
3936	Asymmetric catalysis with 7-ring chelate diphosphines: DIOP, BINAP and conformational mobility. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 1737-1744.	1.8	14
3937	Straightforward synthesis of [(2S,4R)-1-cyclohexyl-4-methylpiperidin-2-yl]methanol and [(2S,4R)-1-cyclohexyl-4-methylpiperidin-2-yl](diphenyl)methanol: novel chiral ligands for the catalytic addition of diethylzinc to benzaldehyde to give rise to an extensive turn in the sense of asymmetric induction. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 2334-2345.	1.8	16
3938	DFT study of the reaction of NO ₂ (2A ₁) with CO(1Î ⁺) mediated by V ⁺ . <i>Computational and Theoretical Chemistry</i> , 2010, 939, 91-96.	1.5	3
3939	Simple charge transfer model for one electron oxidation and reduction processes: Describing reactive sites in benzocarbazolediones and gallates. <i>Computational and Theoretical Chemistry</i> , 2010, 943, 59-64.	1.5	4
3940	Assessment of density functional methods for the study of vanadium and rhenium complexes with thiolato ligands. <i>Computational and Theoretical Chemistry</i> , 2010, 941, 1-9.	1.5	32
3941	Predicting the quality of leaving groups in organic chemistry: Tests against experimental data. <i>Computational and Theoretical Chemistry</i> , 2010, 943, 168-177.	1.5	20
3942	Reaction of Cl with CF ₃ CH ₂ OCHO: A mechanistic and kinetic study. <i>Computational and Theoretical Chemistry</i> , 2010, 944, 124-131.	1.5	2

#	ARTICLE	IF	CITATIONS
3943	Theoretical study of weak CC double bond coordination in a gold (I) catalyst precursor. Computational and Theoretical Chemistry, 2010, 957, 21-25.	1.5	33
3944	The modulation of electronic and optical properties of OXD-X through introduction of the electron-withdrawing groups: A DFT study. Journal of Molecular Graphics and Modelling, 2010, 28, 427-434.	1.3	3
3945	Sulfur hexafluoride plasma surface modification of Gly-Ala and Ala-Gly as Bombyx mori silk model compounds: Mechanism investigations. Journal of Molecular Structure, 2010, 963, 130-136.	1.8	9
3946	Spectroscopic and computational investigation of three Cys-to-Ser mutants of nickel superoxide dismutase: insight into the roles played by the Cys2 and Cys6 active-site residues. Journal of Biological Inorganic Chemistry, 2010, 15, 777-793.	1.1	21
3947	Photodimerizations of hydroxy- and benzoylated 4-azachalcones and quantum chemical investigation of the reactions. Journal of Molecular Modeling, 2010, 16, 1347-1355.	0.8	1
3948	Reactivity versus steric effects in fluorinated ketones as esterase inhibitors: a quantum mechanical and molecular dynamics study. Journal of Molecular Modeling, 2010, 16, 1753-1764.	0.8	9
3949	Incorporation of 2,3-Disubstituted-1,4-Naphthoquinones into the A1 Binding Site of Photosystem I Studied by EPR and ENDOR Spectroscopy. Applied Magnetic Resonance, 2010, 37, 65-83.	0.6	17
3950	Effect of metal ions (Li ⁺ , Na ⁺ , K ⁺ , Mg ²⁺ , Ca ²⁺ , Ni ²⁺ , Cu ²⁺ and Zn ²⁺) and water coordination on the structure and properties of l-histidine and zwitterionic l-histidine. Amino Acids, 2010, 39, 1309-1319.	1.2	60
3951	QSAR and 3D-QSAR studies of the diacyl-hydrazine derivatives containing furan rings based on the density functional theory. Science China Chemistry, 2010, 53, 1322-1331.	4.2	9
3952	Water as dual functional cocatalyst: A theoretical study on the mechanism of direct aldol reaction on water catalyzed by a leucine derivative. Science Bulletin, 2010, 55, 1742-1752.	1.7	12
3953	Temperature Sensitive Nanocapsule of Complex Structural Form for Methane Storage. Nanoscale Research Letters, 2010, 5, 205-210.	3.1	8
3954	Reactions of chlorine atoms and hydroxyl radicals with trichloroethanol: a mechanistic and kinetic study. Journal of Atmospheric Chemistry, 2010, 65, 73-87.	1.4	2
3955	A Comparative Study of the Nonlinear Optical Properties of CdnXn (X: S, Se and Te) Clusters. Journal of Cluster Science, 2010, 21, 591-609.	1.7	4
3956	Synthesis, Crystal Structure, Photophysical Properties, and DFT Calculations of a Bis(tetrathia-calix[4]arene) Tetracadmium Complex. Journal of Cluster Science, 2010, 21, 867-878.	1.7	15
3957	Predictions of hydration free energies from continuum solvent with solute polarizable models: the SAMPL2 blind challenge. Journal of Computer-Aided Molecular Design, 2010, 24, 361-372.	1.3	9
3958	Thermochemistry and crystal lattice energetics of phenyl acridine-9-carboxylates and 9-phenoxy carbonyl-10-methylacridinium trifluoromethanesulphonates. Journal of Thermal Analysis and Calorimetry, 2010, 100, 207-214.	2.0	9
3959	Lattice energetics and thermochemistry of phenyl acridine-9-carboxylates and 9-phenoxy carbonyl-10-methylacridinium trifluoromethanesulphonates. Journal of Thermal Analysis and Calorimetry, 2010, 101, 429-437.	2.0	9
3960	Liposome Damage and Modeling of Fragments of Human Islet Amyloid Polypeptide (IAPP) Support a Two-Step Model of Membrane Destruction. International Journal of Peptide Research and Therapeutics, 2010, 16, 43-54.	0.9	8

#	ARTICLE	IF	CITATIONS
3961	Ab initio and DFT studies of hydrogen bond interactions in difluoroacetic acid dimer. Structural Chemistry, 2010, 21, 643-649.	1.0	10
3962	DFT studies on tautomeric preferences of 1-(pyridin-2-yl)-4-(quinolin-2-yl)butane-2,3-dione in the gas phase and in solution. Structural Chemistry, 2010, 21, 1283-1287.	1.0	4
3963	The Theoretical Study on the Bandgap Change in the Nitrogen-Doped Perovskite-Type Titanium Oxide of SrTiO ₃ . Topics in Catalysis, 2010, 53, 566-570.	1.3	22
3964	The interface structures formation and their effectiveness for enhancement of the phase stability in Ti/Si binary oxide. Materials Chemistry and Physics, 2010, 123, 723-726.	2.0	2
3965	Reaction profiles of the interaction between sarin and acetylcholinesterase and the S203C mutant: Model nucleophiles and QM/MM potential energy surfaces. Chemico-Biological Interactions, 2010, 187, 220-224.	1.7	13
3966	Ab initio and density functional theory studies of the structure, gas phase acidity and aromaticity of tetraselenosquaric acid. Chinese Journal of Chemistry, 2000, 18, 808-814.	2.6	23
3967	Evaluation of a Combined Quantum Chemical Method Used in Calculating O-H Bond Dissociation Enthalpy. Chinese Journal of Chemistry, 2001, 19, 657-661.	2.6	24
3968	Theoretical study on the antioxidant activity of curcumin. Chinese Journal of Chemistry, 2004, 22, 827-830.	2.6	23
3969	DFT Study for the Reduction of N ₂ O(¹ Σ ⁺) with CO(¹ Σ ⁺) Catalyzed by Cr ⁺ . Chinese Journal of Chemistry, 2010, 28, 1363-1368.	2.6	2
3970	Mechanistic Study of the Reaction of Thiol-Containing Enzymes with α,β -Unsaturated Carbonyl Substrates by Computation and Chemoassays. ChemMedChem, 2010, 5, 869-880.	1.6	32
3971	Global Minimum Energy Structure and Spectroscopic Properties of I ₂ ⁺ ...n...H ₂ O Clusters: A Monte Carlo Simulated Annealing Study. ChemPhysChem, 2010, 11, 220-228.	1.0	19
3972	Anion-Dependent Tendency of Di-Long-Chain Quaternary Ammonium Salts to Form Ion Quadruples and Higher Aggregates in Benzene. ChemPhysChem, 2010, 11, 3243-3254.	1.0	36
3973	QM/MM calculation of solvent effects on absorption spectra of guanine. Journal of Computational Chemistry, 2010, 31, 90-106.	1.5	60
3974	Excess electron is trapped in a large single molecular cage C ₆₀ F ₆₀ . Journal of Computational Chemistry, 2010, 31, 195-203.	1.5	49
3975	Atomistic insight into chondroitin-6-sulfate glycosaminoglycan chain through quantum mechanics calculations and molecular dynamics simulation. Journal of Computational Chemistry, 2010, 31, 1670-1680.	1.5	11
3976	Ab Initio and Quantum Chemical Topology studies on the isomerization of HONO to HNO ₂ . Effect of the basis set in QCT. Journal of Computational Chemistry, 2010, 31, 2555-2567.	1.5	6
3977	Comparison of aromatic NH...N, OH...N, and CH...N interactions of alanine using MP2, CCSD, and DFT methods. Journal of Computational Chemistry, 2010, 31, 2874-2882.	1.5	110
3978	QM/MM method for metal-organic interfaces. Journal of Computational Chemistry, 2010, 31, 2955-2966.	1.5	9

#	ARTICLE	IF	CITATIONS
3979	Functionalization of Dinitrogen Using a Historically Significant Ru Complex: A New Life for an Old Complex. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 4716-4719.	1.0	5
3980	Investigation of the Zero-Field Splitting in Six- and Seven-Coordinate Mononuclear Mn ^{II} Complexes with N/O-Based Ligands by Combining EPR Spectroscopy and Quantum Chemistry. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 3658-3665.	1.0	28
3981	Density Functional Theory Studies of [Fe(O)2L]2+: What is the Role of the Spectator Ligand L with Different Coordination Numbers?. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5113-5123.	1.0	4
3982	DFT Study on Tautomerism of Dihydro-1,5-benzodiazepin-2-ones and Dihydro-1,5-benzodiazepine-2-thiones. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 280-291.	1.2	19
3983	Experimental and Theoretical Studies of a One-Flask Synthesis of 3H-1-Benzazepines from 2-Haloanilines and α,β -Unsaturated Ketones. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 2363-2371.	1.2	6
3984	2,2,4,6,7-Pentamethyl-2,3-dihydrobenzofuran-5-methyl (Pbfm) as an Alternative to the Trityl Group for the Side-Chain Protection of Cysteine and Asparagine/Glutamine. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 3631-3640.	1.2	11
3985	Regiospecific Three-Component Access to Fluorescent 2,4-Disubstituted Quinolines via One-Pot Coupling-Addition-Cyclocondensation-Sulfur Extrusion Sequence. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 3516-3524.	1.2	25
3986	Exceptional Superbasicity of Bis(guanidine) Proton Sponges Imposed by the Bis(secododecahedrane) Molecular Scaffold: A Computational Study. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 6563-6572.	1.2	30
3987	Tris(8-hydroxyquinoline-5-sulfonate)aluminum Intercalated Mg-Al Layered Double Hydroxide with Blue Luminescence by Hydrothermal Synthesis. <i>Advanced Functional Materials</i> , 2010, 20, 2848-2856.	7.8	58
3988	Enantioselective Copper-Catalysed Allylic Alkylation of Cinnamyl Chlorides by Grignard Reagents using Chiral Phosphine-Phosphite Ligands. <i>Advanced Synthesis and Catalysis</i> , 2010, 352, 2023-2031.	2.1	50
3989	Brønsted Base-Catalyzed Tandem Isomerization-Michael Reactions of Alkynes: Synthesis of Oxacycles and Azacycles. <i>Advanced Synthesis and Catalysis</i> , 2010, 352, 3373-3379.	2.1	61
3992	Applications of the Cartesian coordinate tensor transfer technique in the simulations of vibrational circular dichroism spectra of oligonucleotides. <i>Chirality</i> , 2010, 22, E96-E114.	1.3	26
3993	Sandwich Compounds of Transition Metals with Cyclopolyenes and Isolobal Boron Analogues. <i>Chemistry - A European Journal</i> , 2010, 16, 2272-2281.	1.7	15
3994	Quinoidal Oligothiophenes: Towards Biradical Ground-State Species. <i>Chemistry - A European Journal</i> , 2010, 16, 470-484.	1.7	74
3995	Persistent Mixed-Valence [(TTF) ₂] ⁺ Dyad of a Chiral Bis(binaphthol)-tetrathiafulvalene (TTF) Derivative. <i>Chemistry - A European Journal</i> , 2010, 16, 8020-8028.	1.7	36
3996	A Definitive Answer to a Bonding Quandary? The Role of One-Electron Resonance Structures in the Bonding of a {Cu ₃ S ₂ } ³⁺ Core. <i>Chemistry - A European Journal</i> , 2010, 16, 2719-2724.	1.7	27
3997	First-Principles Prediction of Nucleophilicity Parameters for π Nucleophiles: Implications for Mechanistic Origin of Mayr's Equation. <i>Chemistry - A European Journal</i> , 2010, 16, 2586-2598.	1.7	41
3998	Electron Attachment to Hydrated Oligonucleotide Dimers: Guanylyl-3',5'-Cytidine and Cytidyl-3',5'-Guanosine. <i>Chemistry - A European Journal</i> , 2010, 16, 5089-5096.	1.7	17

#	ARTICLE	IF	CITATIONS
3999	BF ₃ ·OEt ₂ -Catalyzed Intermolecular Reactions of Vinylidenecyclopropanes with Bis(alkoxyphenyl)methanols: A Novel Cationic 1,4-Aryl Migration Process. Chemistry - A European Journal, 2010, 16, 5163-5172.	1.7	22
4000	Shuangancistrotoresines, Dimeric Naphthylisoquinoline Alkaloids with Three Chiral Biaryl Axes from the Chinese Plant <i>Ancistrocladus tectorius</i> . Chemistry - A European Journal, 2010, 16, 4206-4216.	1.7	38
4001	3,4,5,6-Tetrafluorophenylnitrene: A Ground State Quartet Triradical. Chemistry - A European Journal, 2010, 16, 4496-4506.	1.7	18
4002	Catalytic Asymmetric 1,3-Dipolar Cycloaddition of Iminonitriles. Chemistry - A European Journal, 2010, 16, 5286-5291.	1.7	55
4003	Ir-Catalysed Asymmetric Allylic Substitutions with Cyclometalated (Phosphoramidite)Ir Complexes: Resting States, Catalytically Active (Allyl)Ir Complexes and Computational Exploration. Chemistry - A European Journal, 2010, 16, 6601-6615.	1.7	82
4004	Heteroheptacenes with Fused Thiophene and Pyrrole Rings. Chemistry - A European Journal, 2010, 16, 5119-5128.	1.7	48
4005	Transition States and Origins of 1,4-Asymmetric Induction in Alkylations of 2,2,6-Trialkylpiperidine Enamines. Chemistry - A European Journal, 2010, 16, 6310-6316.	1.7	7
4006	Comparison of Thiophene-Pyrrole Oligomers with Oligothiophenes: A Joint Experimental and Theoretical Investigation of Their Structural and Spectroscopic Properties. Chemistry - A European Journal, 2010, 16, 6866-6876.	1.7	27
4007	(2-Tolylsulfinyl)benzyl Halides as Efficient Precursors of Optically Pure trans-2,3-Disubstituted Aziridines. Chemistry - A European Journal, 2010, 16, 9874-9883.	1.7	31
4008	Demonstration of π -Aromaticity in Planar Metallacycles. Chemistry - A European Journal, 2010, 16, 7843-7851.	1.7	93
4009	1,4-Addition of Bis(iodozincio)methane to α,β -Unsaturated Ketones: Chemical and Theoretical/Computational Studies. Chemistry - A European Journal, 2010, 16, 10474-10481.	1.7	17
4010	High-Yielding Synthesis of the Anti-Influenza Neuraminidase Inhibitor (A) Oseltamivir by Two One-Pot Sequences. Chemistry - A European Journal, 2010, 16, 12616-12626.	1.7	138
4011	Electron Attachment to a Hydrated DNA Duplex: The Dinucleoside Phosphate Deoxyguanylyl-3',5'-Deoxycytidine. Chemistry - A European Journal, 2010, 16, 13155-13162.	1.7	13
4012	(2,1-Indenofluorene Derivatives: Syntheses, X-Ray Structures, Optical and Electrochemical Properties. Chemistry - A European Journal, 2010, 16, 13646-13658.	1.7	52
4016	Highly Enantioselective Recognition of Structurally Diverse α -Hydroxycarboxylic Acids using a Fluorescent Sensor. Angewandte Chemie - International Edition, 2010, 49, 602-606.	7.2	115
4017	Charge Density Distribution in a Metallaphosphane. Angewandte Chemie - International Edition, 2010, 49, 2422-2426.	7.2	30
4018	Water as an Oxygen Source: Synthesis, Characterization, and Reactivity Studies of a Mononuclear Nonheme Manganese(IV) Oxo Complex. Angewandte Chemie - International Edition, 2010, 49, 8190-8194.	7.2	90
4019	Degradation of poly(ethylene glycol) by electrolysis during the Cu electroplating: A combined experimental and density functional theory study. Journal of Applied Polymer Science, 2010, 117, 2083-2089.	1.3	23

#	ARTICLE	IF	CITATIONS
4020	Electron predators are hydrogen atom traps. Effects of aryl groups on N=C± bond dissociations of peptide radicals. <i>Journal of Mass Spectrometry</i> , 2010, 45, 1280-1290.	0.7	12
4021	DFT theoretical studies of antipyrine Schiff bases as corrosion inhibitors. <i>Materials and Corrosion - Werkstoffe Und Korrosion</i> , 2010, 61, 709-714.	0.8	35
4022	Kinetics of the hydrogen abstraction R ₂ OH + H → R ₂ O + H ₂ reaction class. <i>International Journal of Chemical Kinetics</i> , 2010, 42, 414-429.	1.0	21
4023	Vibrational spectra of phenyl acridine-9-carboxylates and their 10-methylated cations: A theoretical and experimental study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 75, 1546-1551.	2.0	1
4024	Electronic spectra of oxocomplexes of Re(V) with thiolato ligands. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 76, 348-355.	2.0	8
4025	The vibrational spectra of 1,3-dithiane-1-oxide and 1,3-dithia-1-oxocyclohept-5-ene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 77, 6-10.	2.0	0
4026	Classical trajectories and RRKM modeling of collisional excitation and dissociation of benzylammonium and tert-butyl benzylammonium ions in a quadrupole-hexapole-quadrupole tandem mass spectrometer. <i>Journal of the American Society for Mass Spectrometry</i> , 2010, 21, 425-439.	1.2	13
4027	Backbone and side-chain specific dissociations of <i>z</i> ions from non-tryptic peptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2010, 21, 1279-1295.	1.2	47
4028	Conformational preferences of sterically congested 2-imidazolidinone using X-ray analysis and computational studies. Part 1: Trans-1-acetyl-4,5-di-tert-butyl-2-imidazolidinone. <i>Journal of Molecular Structure</i> , 2010, 969, 145-154.	1.8	6
4029	Theoretical and experimental study on the reactions between 3,5-di-O-p-toluoyl-d-2-deoxyribose chloride and alcohols. <i>Journal of Molecular Structure</i> , 2010, 977, 1-5.	1.8	2
4030	On the magnetic and thermodynamic properties of Americium-II: A hybrid density functional theoretic study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010, 374, 4704-4712.	0.9	5
4031	Electronic characterization of all-thiophene conducting dendrimers: Molecules and assemblies. <i>Polymer</i> , 2010, 51, 308-315.	1.8	10
4032	Microscopic details of the sensing ability of 15-crown-5-ether functionalized poly(bithiophene). <i>Polymer</i> , 2010, 51, 4267-4272.	1.8	11
4033	Theoretical prediction of a peptide binding to major histocompatibility complex II. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 29, 240-245.	1.3	6
4034	Spectral, structural and DFT studies of platinum group metal 3,6-bis(2-pyridyl)-4-phenylpyridazine complexes and their ligand bonding modes. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 707-716.	0.8	19
4035	Silyl-substituted germenenes. The reactions of germenenes generated thermally from acyltris(trimethylsilyl)germane with conjugated enones. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 1663-1674.	0.8	6
4036	New ferrocenyl-substituted heterocycles. Formation under Biginelli conditions, DFT modelling, and structure determination. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 1852-1857.	0.8	17
4037	Synthesis and thermal behavior of cis- and trans-1-tert-butyl-4,5-dimethyl-2-phenyl-2-(trimethylsilyloxy)-1-(trimethylsilyl)-1-silacyclohex-4-ene. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2499-2505.	0.8	1

#	ARTICLE	IF	CITATIONS
4038	Electrophilic ipso-iodination of silylated arylboronic acids. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2635-2643.	0.8	13
4039	The mechanisms of ROS-photogeneration by berberine, a natural isoquinoline alkaloid. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2010, 99, 154-156.	1.7	12
4040	Enhancing the light driven modulation of the refractive index in organic photochromic materials: A quantum chemical strategy. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2010, 214, 61-68.	2.0	10
4041	Adsorption of hydrogen atoms onto the exterior wall of carbon nanotubes and their thermodynamics properties. <i>International Journal of Hydrogen Energy</i> , 2010, 35, 4543-4553.	3.8	18
4042	Calculation of DFT molecular properties using the -Integral method. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2010, 389, 5208-5215.	1.2	6
4043	Hydrogenation of carbon-heteroatom unsaturated bonds: An assessment of consistency of density functional methods. <i>Journal of Molecular Catalysis A</i> , 2010, 324, 97-103.	4.8	3
4044	Rhodium(I) mediated arylation of aldehydes with arylboronic acids under base and water free conditions: A computational study. <i>Journal of Molecular Catalysis A</i> , 2010, 324, 24-30.	4.8	5
4045	Computational investigations of the stereoselectivities of proline-related catalysts for aldol reactions. <i>Journal of Molecular Catalysis A</i> , 2010, 324, 31-38.	4.8	41
4046	Trans effects in the Heck reaction. A model study. <i>Journal of Molecular Catalysis A</i> , 2010, 328, 108-113.	4.8	18
4047	Spectroscopic and theoretical study on inclusion complexation of beta-cyclodextrin with permethrin. <i>Journal of Molecular Structure</i> , 2010, 981, 194-203.	1.8	63
4048	Experimental and theoretical analysis of polymerization reaction process on the polydopamine membranes and its corrosion protection properties for 304 Stainless Steel. <i>Journal of Molecular Structure</i> , 2010, 982, 152-161.	1.8	190
4049	The effect of substitution on reorganization energy and charge mobility in metal free phthalocyanine. <i>Chemical Physics</i> , 2010, 367, 7-19.	0.9	25
4050	Theoretical study of the low-lying excited states of -carotene isomers by a multireference configuration interaction method. <i>Chemical Physics</i> , 2010, 373, 98-103.	0.9	32
4051	Infrared spectroscopy of (CHF ₂ Cl) ₂ and CHF ₂ Cl·H ₂ O complex in Xe matrix. <i>Chemical Physics</i> , 2010, 369, 82-90.	0.9	13
4052	A study on the synthesis of structural analogs of bis-indole alkaloid caulerpin: a step-by-step synthesis of a cyclic indole-tetramer. <i>Tetrahedron</i> , 2010, 66, 1902-1910.	1.0	27
4053	New 3-vinylation products of indole and investigation of its Diels-Alder reactivity: synthesis of unusual Morita-Baylis-Hillman-type products. <i>Tetrahedron</i> , 2010, 66, 3214-3221.	1.0	7
4054	Two isolated intermediates of the Tröger's base: synthesis and mechanism. <i>Tetrahedron</i> , 2010, 66, 3405-3409.	1.0	10
4055	The generation of diazirinone: a computational study. <i>Tetrahedron Letters</i> , 2010, 51, 3266-3268.	0.7	8

#	ARTICLE	IF	CITATIONS
4056	Theoretical study on the reaction of Be(3P) with methane. Computational and Theoretical Chemistry, 2010, 942, 66-70.	1.5	2
4057	Electronic band structure of alternating fluorene-oxadiazole conjugated copolymer – A 1D solid-state DFT study. Computational and Theoretical Chemistry, 2010, 944, 146-155.	1.5	8
4058	Computational study on the conformations of mitragynine and mitragynaline. Computational and Theoretical Chemistry, 2010, 945, 57-63.	1.5	7
4059	Quantum chemical studies on chameleonic ligand and its grid-type copper(I) and zinc(II) complexes. Computational and Theoretical Chemistry, 2010, 949, 82-87.	1.5	2
4060	In silico assessment of drug substances chemical stability. Computational and Theoretical Chemistry, 2010, 954, 75-79.	1.5	41
4061	A molecular orbital treatment of piroxicam and its M ²⁺ -complexes: The change of the drug configuration in a time of bond formation. Computational and Theoretical Chemistry, 2010, 951, 14-20.	1.5	15
4062	Quantum chemical calculations of the homogeneous, unimolecular, gas-phase elimination kinetics of primary alkyl acetates and (dimethylamino)alkyl acetates: Neighboring group participation in 4-(dimethylamino)-1-butyl acetate. Computational and Theoretical Chemistry, 2010, 952, 46-55.	1.5	4
4063	Theoretical study on the reaction of Nb ⁺ with COS in the gas phase. Computational and Theoretical Chemistry, 2010, 953, 39-46.	1.5	0
4064	On the dissociation of DNA enhanced by radical cations. Computational and Theoretical Chemistry, 2010, 955, 152-157.	1.5	1
4065	Competitive activation of C–H and C–X bonds in gas phase reaction of Pt with CH ₂ FCl: A DFT study. Computational and Theoretical Chemistry, 2010, 959, 8-14.	1.5	9
4066	The nature of hydrogen bonds with divalent selenium compounds. Computational and Theoretical Chemistry, 2010, 959, 1-7.	1.5	23
4067	A comparative DFT study of atomic and molecular oxygen adsorption on neutral and negatively charged Pd _x Cu _{3-x} (x=0–3) nano-clusters. Computational and Theoretical Chemistry, 2010, 959, 15-21.	1.5	16
4068	Computational simulation of the molecular structure of some triazoles as inhibitors for the corrosion of metal surface. Computational and Theoretical Chemistry, 2010, 959, 66-74.	1.5	243
4069	Density functional study of the nitrosamine–formic acid and nitrosamine–formamide interactions. Computational and Theoretical Chemistry, 2010, 960, 15-21.	1.5	2
4070	Density functional theory calculations of the gas-phase elimination kinetics of 2-(dimethylamino)ethyl chloride and ethyl chloride. Computational and Theoretical Chemistry, 2010, 961, 55-61.	1.5	3
4071	C–N bond dissociation energies: An assessment of contemporary DFT methodologies. Computational and Theoretical Chemistry, 2010, 961, 97-100.	1.5	25
4072	Theoretical characterization of hole mobility in N,N'-diphenyl-N,N'-bis(3-methylphenyl)-(1,1'-biphenyl)-4,4'-diamine. Computational and Theoretical Chemistry, 2010, 962, 80-84.	1.5	9
4073	Morphology and growing of nanometric multilayered films formed by alternated layers of poly(3,4-ethylenedioxythiophene) and poly(N-methylpyrrole). Thin Solid Films, 2010, 518, 4203-4210.	0.8	31

#	ARTICLE	IF	CITATIONS
4074	Lattice and internal relaxation of ZnO thin film under in-plane strain. <i>Thin Solid Films</i> , 2010, 519, 378-384.	0.8	12
4075	First-principle study of full Heusler using PBE0 hybrid functional. <i>Solid State Communications</i> , 2010, 150, 1501-1504.	0.9	24
4076	The pH effect on black spots in surface finish: Electroless nickel immersion gold. <i>Applied Surface Science</i> , 2010, 257, 56-61.	3.1	31
4077	Scope and reaction mechanism of an aerobic oxidative alkyne homocoupling catalyzed by a di-copper-substituted silicotungstate. <i>Catalysis Today</i> , 2010, 157, 359-363.	2.2	25
4078	Methyl and methane elimination in the gas phase reaction of zirconium atom with 2-butyne: A DFT study. <i>Chinese Chemical Letters</i> , 2010, 21, 1501-1504.	4.8	0
4079	Ab initio investigation on the nonlinear optical properties of Cd _n Ten (n=1-10) clusters. <i>Chemical Physics</i> , 2010, 367, 152-159.	0.9	9
4080	Determination of enthalpy of formation of methyl and ethyl esters of fatty acids. <i>Chemistry and Physics of Lipids</i> , 2010, 163, 172-181.	1.5	33
4081	Theoretical study of the gas phase reaction of methyl acetate with the hydroxyl radical: Structures, mechanisms, rates and temperature dependencies. <i>Chemical Physics Letters</i> , 2010, 490, 116-122.	1.2	26
4082	Studies on adsorption of carnosine on silver nanoparticles by SERS. <i>Chemical Physics Letters</i> , 2010, 491, 59-64.	1.2	33
4083	Spin-flip time dependent density functional theory for singlet-triplet splittings in $\dot{I}f, \dot{I}f$ -biradicals. <i>Chemical Physics Letters</i> , 2010, 491, 132-135.	1.2	35
4084	Protocovalent N-O bonding in methyl nitrite (CH ₃ ONO) and ethyl nitrite (C ₂ H ₅ ONO). Topological analysis of the electron localization function (ELF) and electron localizability indicator (ELI-D) functions. <i>Chemical Physics Letters</i> , 2010, 493, 392-398.	1.2	7
4085	Theoretical study on the atmospheric formation of cis and trans-OSSO complexes. <i>Chemical Physics Letters</i> , 2010, 494, 315-322.	1.2	12
4086	Theoretical study on the mechanism of S ₂ + O ₂ reaction. <i>Chemical Physics Letters</i> , 2010, 497, 1-6.	1.2	9
4087	Theoretical investigation for the reaction of N ₂ O with CO catalyzed by MO ⁺ (M=Ru, Os). <i>Chemical Physics Letters</i> , 2010, 498, 245-252.	1.2	5
4088	Theoretical study on the formation of tetraoxygen conformational isomerism in the CO ₂ with O ₃ reaction. <i>Chemical Physics Letters</i> , 2010, 499, 51-55.	1.2	5
4089	Divide-and-conquer self-consistent field calculation for open-shell systems: Implementation and application. <i>Chemical Physics Letters</i> , 2010, 500, 172-177.	1.2	43
4090	Molecular modeling study of binding site selectivity of TQMP to G-quadruplex DNA. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 983-991.	2.6	16
4091	Conformational polymorphism in a Schiff-base macrocyclic organic ligand: an experimental and theoretical study. <i>Acta Crystallographica Section B: Structural Science</i> , 2010, 66, 527-543.	1.8	13

#	ARTICLE	IF	CITATIONS
4092	The relationship between catalyst precursors and chain end groups in homogeneous propene polymerization catalysis. <i>Journal of Polymer Science Part A</i> , 2010, 48, 699-708.	2.5	16
4093	A DFT study on the mechanisms for gas phase reaction of yttrium with propene. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 768-775.	0.9	7
4094	Chiral recognition in self-assembly complexes of diketopiperazine derivatives. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 1155-1172.	0.9	11
4095	Theoretical mechanisms of the superoxide radical anion catalyzed by the copper-zinc superoxide dismutase. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1394-1401.	1.0	14
4096	CASSCF/CASPT2 analysis of the fragmentation of H ₂ on a Pd ₄ cluster. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 558-562.	1.0	19
4097	Approach to potential energy surfaces by neural networks. A review of recent work. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 432-445.	1.0	10
4098	Models for the adsorption and self-assembly of ethanol and 1-decanethiol on Au(111) surfaces. A comparative study by computer simulation. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 293-306.	1.0	0
4099	Molecular excitation spectra by TDDFT with the nonadiabatic exact exchange kernel. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2202-2220.	1.0	23
4100	Spectroscopic and photophysical properties of dicopper(I) metallocyclophanes. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 3061-3071.	1.0	1
4101	Direct transformation of graphene to fullerene. <i>Nature Chemistry</i> , 2010, 2, 450-453.	6.6	361
4102	Quantum Control of Laser-driven Chiral Molecular Motors. , 0, , .		0
4103	Facile Synthesis and Preferred Conformation Analysis of Cyclododeceno[b]indene. <i>Molecules</i> , 2010, 15, 699-708.	1.7	0
4105	Anisotropy in electronic, optical, and mechanical properties of superhard body-centered tetragonal C4 phase of carbon. <i>Applied Physics Letters</i> , 2010, 97, 061910.	1.5	17
4106	Identification of a Tri-Iron(III), Tri-Citrate Complex in the Xylem Sap of Iron-Deficient Tomato Resupplied with Iron: New Insights into Plant Iron Long-Distance Transport. <i>Plant and Cell Physiology</i> , 2010, 51, 91-102.	1.5	235
4107	The Refinement of Self-Trapped Excitons Structure in CaF ₂ and SrF ₂ Crystals: An Ab Initio Study. <i>IEEE Transactions on Nuclear Science</i> , 2010, 57, 1200-1203.	1.2	6
4108	A Quasirelativistic Two-component Density Functional and Hartree-Fock Program. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 413-426.	1.4	41
4109	Density-Functional Theory with Orbital-Dependent Functionals: Exact-exchange Kohn-Sham and Density-Functional Response Methods. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 325-342.	1.4	16
4110	Energy band structure calculations based on screened Hartree-Fock exchange method: Si, AlP, AlAs, GaP, and GaAs. <i>Journal of Chemical Physics</i> , 2010, 132, 224105.	1.2	48

#	ARTICLE	IF	CITATIONS
4111	Doubly π -Functionalized Zinc(II) Porphyrin-Sensitized TiO ₂ Solar Cells. Journal of the Chinese Chemical Society, 2010, 57, 1111-1118.	0.8	12
4112	Random phase approximation correlation energies with exact Kohn-Sham exchange. Molecular Physics, 2010, 108, 359-372.	0.8	121
4113	XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. Journal of Chemical Physics, 2010, 132, 194105.	1.2	40
4114	Is the oxygen π -side-on, or π -end-on, and functional, in peroxy radicals with magnetically equivalent oxygen atoms?. Canadian Journal of Chemistry, 2010, 88, 1053-1056.	0.6	3
4115	Validation of density-functional versus density-functional+U approaches for oxide ultrathin films. Journal of Chemical Physics, 2010, 132, 124703.	1.2	47
4116	Ab initio static and molecular dynamics study of the absorption spectra of the 4-styrylpyridine photoswitch in its cis and trans forms. Physical Chemistry Chemical Physics, 2010, 12, 6107.	1.3	20
4117	Alignment of defect levels and band edges through hybrid functionals: Effect of screening in the exchange term. Physical Review B, 2010, 81, .	1.1	124
4118	A first principles study of fluorescence quenching in rhodamine B dimers: how can quenching occur in dimeric species?. Physical Chemistry Chemical Physics, 2010, 12, 11238.	1.3	103
4119	Trypsin-Catalyzed Cross-Linking of γ -Triethoxysilyl-Terminated Polydimethylsiloxane: An Experimental and Computational Approach. ACS Symposium Series, 2010, , 47-57.	0.5	2
4120	On the conditions for enhanced transport through molecular junctions based on metal centres ligated by pairs of pyridazino-derived ligands. Molecular Physics, 2010, 108, 2591-2599.	0.8	2
4121	A DFT study on the catalytic mechanism of UDP-glucose dehydrogenase. Canadian Journal of Chemistry, 2010, 88, 804-814.	0.6	2
4122	DFT + U study of defects in bulk rutile TiO ₂ . Journal of Chemical Physics, 2010, 133, 144708.	1.2	126
4123	Basis set dependence of the doubly hybrid XYG3 functional. Journal of Chemical Physics, 2010, 133, 104105.	1.2	41
4124	Link atom bond length effect in ONIOM excited state calculations. Journal of Chemical Physics, 2010, 133, 054104.	1.2	10
4125	Branched nanotrees with immobilized acetylcholine esterase for nanobiosensor applications. Nanotechnology, 2010, 21, 055102.	1.3	10
4126	B3LYP Study on Reduction Mechanisms from to at the Catalytic Sites of Fully Reduced and Mixed-Valence Bovine Cytochrome Oxidases. Bioinorganic Chemistry and Applications, 2010, 2010, 1-18.	1.8	6
4127	Insight into the Strong Antioxidant Activity of Deinoxanthin, a Unique Carotenoid in Deinococcus Radiodurans. International Journal of Molecular Sciences, 2010, 11, 4506-4510.	1.8	29
4128	A divide and conquer real space finite-element Hartree-Fock method. Journal of Chemical Physics, 2010, 132, 034101.	1.2	29

#	ARTICLE	IF	CITATIONS
4129	Assignment of near-edge x-ray absorption fine structure spectra of metalloporphyrins by means of time-dependent density-functional calculations. <i>Journal of Chemical Physics</i> , 2010, 133, 054703.	1.2	59
4130	Negative ion photoelectron spectroscopy of the copper-aspartic acid anion and its hydrated complexes. <i>Journal of Chemical Physics</i> , 2010, 133, 084303.	1.2	1
4131	Many-electron self-interaction and spin polarization errors in local hybrid density functionals. <i>Journal of Chemical Physics</i> , 2010, 133, 134116.	1.2	83
4132	Range-dependent adiabatic connections. <i>Journal of Chemical Physics</i> , 2010, 133, 164112.	1.2	30
4133	Frozen density embedding with hybrid functionals. <i>Journal of Chemical Physics</i> , 2010, 133, 164111.	1.2	49
4134	Communication: Systematic shifts of the lowest unoccupied molecular orbital peak in x-ray absorption for a series of 3d metal porphyrins. <i>Journal of Chemical Physics</i> , 2010, 133, 151103.	1.2	33
4135	Prediction of Excitation Energies for Conjugated Oligomers and Polymers from Time-Dependent Density Functional Theory. <i>Materials</i> , 2010, 3, 3430-3467.	1.3	3
4136	Modeling of spectral signatures using ab initio calculations. <i>Proceedings of SPIE</i> , 2010, , .	0.8	0
4137	Novel semiconductors based on functionalized benzo[d,d']thieno[3,2- b ;4,5- b']dithiophenes (BTDTs) and the effects of thin film growth conditions on organic field effect transistor performance. <i>Proceedings of SPIE</i> , 2010, , .	0.8	0
4138	Electronic excitation energies in solution at equation of motion CCSD level within a state specific polarizable continuum model approach. <i>Journal of Chemical Physics</i> , 2010, 132, 084102.	1.2	47
4139	Insights into the ultraviolet spectrum of liquid water from model calculations. <i>Journal of Chemical Physics</i> , 2010, 132, 244307.	1.2	22
4140	Rotationally resolved electronic spectroscopy of 5-methoxyindole. <i>Journal of Chemical Physics</i> , 2010, 133, 024303.	1.2	23
4141	Rung 3.5 density functionals. <i>Journal of Chemical Physics</i> , 2010, 133, 104103.	1.2	36
4142	Predicting Rate Constants for Nucleophilic Reactions of Amines with Diarylcarbenium Ions Using an ONIOM Method. <i>Chinese Journal of Chemical Physics</i> , 2010, 23, 669-674.	0.6	2
4143	A TDDFT Study of the Fluorescence Properties of Three Alkoxyridylindolizine Derivatives. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7094-7101.	1.1	30
4144	Lithium Cadmate-Mediated Deprotonative Metalation of Anisole: Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 3117-3120.	1.7	21
4145	Effect of Waters of Crystallization on Terahertz Spectra: Anhydrous Oxalic Acid and Its Dihydrate. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7127-7138.	1.1	60
4146	Screened exchange density functional applied to solids. <i>Physical Review B</i> , 2010, 82, .	1.1	189

#	ARTICLE	IF	CITATIONS
4148	Modeling of Amorphous Polyaniline Emeraldine Base. <i>Journal of Physical Chemistry B</i> , 2010, 114, 9771-9777.	1.2	12
4149	Accurate calculation and modeling of the adiabatic connection in density functional theory. <i>Journal of Chemical Physics</i> , 2010, 132, 164115.	1.2	86
4150	Quantum chemical dissection of the classic terpinyl/pinyl/bornyl/camphyl cation conundrum—the role of pyrophosphate in manipulating pathways to monoterpenes. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 4589.	1.5	73
4151	Enantioselective Synthesis of Axially Chiral Biaryls by the Pd-Catalyzed Suzuki–Miyaura Reaction: Substrate Scope and Quantum Mechanical Investigations. <i>Journal of the American Chemical Society</i> , 2010, 132, 11278-11287.	6.6	249
4152	Single molecule detection using graphene electrodes. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2010, 43, 115101.	0.6	22
4153	Intersulfur Distance Is a Key Factor in Tuning Disulfide Radical Anion Vertical UV–Visible Absorption. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 581-586.	2.1	6
4154	Joint Experimental and DFT Study of the Gas-Phase Unimolecular Elimination Kinetic of Methyl Trifluoropyruvate. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7892-7897.	1.1	4
4155	Effects of Urea, Tetramethyl Urea, and Trimethylamine <i>N</i> -Oxide on Aqueous Solution Structure and Solvation of Protein Backbones: A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 557-568.	1.2	159
4156	Selective Activation of the <i>ortho</i> -C–F Bond in Pentafluoropyridine by Zerovalent Nickel: Reaction via a Metallophosphorane Intermediate Stabilized by Neighboring Group Assistance from the Pyridyl Nitrogen. <i>Organometallics</i> , 2010, 29, 1824-1831.	1.1	87
4157	Controlling Electron Transfer in Donor–Bridge–Acceptor Molecules Using Cross-Conjugated Bridges. <i>Journal of the American Chemical Society</i> , 2010, 132, 15427-15434.	6.6	144
4158	Accurate Estimation of the One-Electron Reduction Potentials of Various Substituted Quinones in DMSO and CH ₃ CN. <i>Journal of Organic Chemistry</i> , 2010, 75, 5037-5047.	1.7	82
4159	Bridged Photochromic Diarylethenes Investigated by Ultrafast Absorption Spectroscopy: Evidence for Two Distinct Photocyclization Pathways. <i>Journal of the American Chemical Society</i> , 2010, 132, 7379-7390.	6.6	62
4160	Room-Temperature Phosphorescence of the DNA Monomer Analogue 4-Thiothymidine in Aqueous Solutions after UVA Excitation. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2239-2243.	2.1	81
4161	Quantum Chemical Modeling of the Cardiolipin Headgroup. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4375-4387.	1.1	21
4162	Novel Semiconductors Based on Functionalized Benzo[<i>d</i>], <i>d</i> ’-thieno[3,2- <i>b</i>];4,5- <i>b</i> ’-dithiophenes and the Effects of Thin Film Growth Conditions on Organic Field Effect Transistor Performance. <i>Chemistry of Materials</i> , 2010, 22, 5031-5041.	3.2	45
4163	Sulfoxidation with hydrogen peroxide catalyzed by [SeO ₄ {WO(O ₂) ₂ } ₂] ²⁻ . <i>Dalton Transactions</i> , 2010, 39, 5509.	1.6	53
4164	Function-Oriented Synthesis of Simplified Caprazamycins: Discovery of Oxazolidine-Containing Uridine Derivatives as Antibacterial Agents against Drug-Resistant Bacteria. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 3793-3813.	2.9	79
4165	Extending the reliability and applicability of B3LYP. <i>Chemical Communications</i> , 2010, 46, 3057.	2.2	196

#	ARTICLE	IF	CITATIONS
4166	Theoretical Studies of the Electronic Structure of Compounds of the Actinide Elements. , 2010, , 1893-2012.		8
4167	Adiabatic connection at negative coupling strengths. Physical Review A, 2010, 81, .	1.0	13
4168	Torsionally Controlled Electronic Coupling in Mixed-Valence Oxodimolybdenum Nitrosyl Scorpionates - a DFT Study. Inorganic Chemistry, 2010, 49, 7676-7684.	1.9	14
4169	Realistic many-body models for manganese monoxide under pressure. Physical Review B, 2010, 81, .	1.1	33
4170	The inactivation of lipid peroxide radical by quercetin. A theoretical insight. Physical Chemistry Chemical Physics, 2010, 12, 7662.	1.3	92
4171	Global Hybrid Functionals: A Look at the Engine under the Hood. Journal of Chemical Theory and Computation, 2010, 6, 3688-3703.	2.3	87
4172	Synthesis and Mechanistic Studies of Organic Chromophores with Different Energy Levels for p-Type Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2010, 114, 4738-4748.	1.5	174
4173	Homoselenocysteine " An oxygen or selenium acid in the gas phase?. Canadian Journal of Chemistry, 2010, 88, 744-753.	0.6	2
4174	Prediction of ⁵⁷ Fe Mössbauer Parameters by Density Functional Theory: A Benchmark Study. Journal of Chemical Theory and Computation, 2010, 6, 3735-3749.	2.3	54
4175	Insights into Photoinduced Electron Transfer Between [Ru(mptpy) ₂] ⁴⁺ (mptpy) Tj ETQq1 1 0.784314 rgBT Computational and Experimental Studies. Journal of Physical Chemistry A, 2010, 114, 6284-6297.	1.1	27
4176	GW method with the self-consistent Sternheimer equation. Physical Review B, 2010, 81, .	1.1	122
4178	Quantitative structure-reactivity modeling of copper-catalyzed atom transfer radical polymerization. Polymer Chemistry, 2010, 1, 922.	1.9	15
4179	Theoretical predictions of a highly reactive non-heme Fe(IV)O complex with a high-spin ground state. Chemical Communications, 2010, 46, 4511.	2.2	23
4180	High Yield Access to Silylene RSiCl (R = PhC(N<i>t</i>Bu) ₂) and Its Reactivity toward Alkyne: Synthesis of Stable Disilacyclobutene. Journal of the American Chemical Society, 2010, 132, 1123-1126.	6.6	271
4181	Range-separated local hybrids. Journal of Chemical Physics, 2010, 132, 224106.	1.2	41
4182	On the TD-DFT Accuracy in Determining Single and Double Bonds in Excited-State Structures of Organic Molecules. Journal of Physical Chemistry A, 2010, 114, 13402-13410.	1.1	76
4183	Stereocontrolled Syntheses of (âˆ“) -Cubebol and (âˆ“) -10-Epicubebol Involving Intramolecular Cyclopropanation of Î±-Lithiated Epoxides. Journal of Organic Chemistry, 2010, 75, 2157-2168.	1.7	39
4184	Failure of Conventional Density Functionals for the Prediction of Molecular Crystal Polymorphism: A Quantum Monte Carlo Study. Journal of Physical Chemistry Letters, 2010, 1, 1789-1794.	2.1	61

#	ARTICLE	IF	CITATIONS
4185	DFT studies on catalytic properties of isolated and carbon nanotube supported Pd ₉ cluster : Part II. Hydro-isomerization of butene isomers. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1323-1330.	1.3	21
4186	Theoretical Prediction of Stable Noble-Gas Anions XeNO ₂ ⁺ and XeNO ₃ ⁺ with very Short Xenon-Nitrogen Bond Lengths. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9359-9367.	1.1	22
4187	Hybrid functionals within the all-electron FLAPW method: Implementation and applications of PBE0. <i>Physical Review B</i> , 2010, 81, .	1.1	48
4188	Study of Proton Coupled Electron Transfer in a Biomimetic Dimanganese Water Oxidation Catalyst with Terminal Water Ligands. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2395-2401.	2.3	52
4189	Characterization of Proton Coupled Electron Transfer in a Biomimetic Oxomanganese Complex: Evaluation of the DFT B3LYP Level of Theory. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 755-760.	2.3	61
4190	On the Electronic and Structural Properties of Tri-Niobium Oxide Clusters Nb ₃ O _n ⁺ (n = 3-8): Photoelectron Spectroscopy and Density Functional Calculations. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5958-5966.	1.1	45
4191	Alignment and Relaxation Dynamics of Dye Molecules in Host-Guest Inclusion Compounds As Probed by Dielectric Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6956-6963.	1.1	12
4192	Novel Intramolecular Energy Transfer Probe for the Detection of Benzo[a]pyrene Metabolites in a Homogeneous Competitive Fluorescence Immunoassay. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1666-1673.	1.2	18
4193	Compelling Computational Evidence for the Concerted Cyclization of the ABC Rings of Hopene from Protonated Squalene. <i>Journal of the American Chemical Society</i> , 2010, 132, 17111-17117.	6.6	44
4194	The Histidine Effect. Electron Transfer and Capture Cause Different Dissociations and Rearrangements of Histidine Peptide Cation-Radicals. <i>Journal of the American Chemical Society</i> , 2010, 132, 10728-10740.	6.6	55
4195	Insights into the Mechanism of O ₂ Formation and Release from the Mn ₄ O ₄ L ₆ C ₆₀ -Cluster. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11417-11424.	1.1	27
4196	n-Alkane Isodesmic Reaction Energy Errors in Density Functional Theory Are Due to Electron Correlation Effects. <i>Organic Letters</i> , 2010, 12, 4670-4673.	2.4	57
4197	Theoretical Study of the O ₂ Interaction with a Tetrahedral Al ₄ Cluster. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11746-11750.	1.1	19
4198	Geometry Dependence of the Ring-Opening E2 Reaction in Lactones. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1392-1397.	1.1	4
4199	Synthesis and Structural and Computational Studies of a Conformationally Locked (l ¹ -Perfluoroalkylidene)(l ² -alkene) Transition Metal Complex: Ir(Cp*)(CFCF ₃)(C ₂ H ₄). <i>Organometallics</i> , 2010, 29, 1942-1947.	1.1	23
4200	Hydrido-Ruthenium Cluster Complexes as Models for Reactive Surface Hydrogen Species of Ruthenium Nanoparticles. Solid-State ² H NMR and Quantum Chemical Calculations. <i>Journal of the American Chemical Society</i> , 2010, 132, 11759-11767.	6.6	44
4201	Photoelectron Imaging and Theoretical Studies of Group 11 Cyanides MCN (M = Cu, Ag, Au). <i>Journal of Physical Chemistry A</i> , 2010, 114, 12839-12844.	1.1	29
4202	Ambipolar Charge Transport in ±-Oligofurans: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20436-20442.	1.5	64

#	ARTICLE	IF	CITATIONS
4203	DFT Study on the Mechanism of Amides to Aldehydes Using Cp ₂ Zr(H)Cl. <i>Organometallics</i> , 2010, 29, 42-51.	1.1	22
4204	Reply to "Comment on "Enthalpy Difference between Conformations of Normal Alkanes: Raman Spectroscopy Study of <i>n</i> -Pentane and <i>n</i> -Butane". <i>Journal of Physical Chemistry A</i> , 2010, 114, 6729-6730.	1.1	4
4205	Is There Symmetry Breaking in the First Excited Singlet State of 2-Pyridone Dimer?. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6897-6903.	1.1	11
4206	Folding a Polymer via Two-Point Interaction with an External Folding Agent: Use of H-Bonding and Charge-Transfer Interactions. <i>Macromolecules</i> , 2010, 43, 3183-3192.	2.2	28
4207	Calculation of Magnetic Couplings with Double-Hybrid Density Functionals. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1201-1204.	2.1	27
4208	Structural Study of Selected Polyhalogenated Benzimidazoles (Protein Kinase CK2 Inhibitors) by Nuclear Quadrupole Double Resonance, X-ray, and Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2010, 114, 563-575.	1.1	26
4209	Discrimination of Chiral Solids: A Terahertz Spectroscopic Investigation of <i>l</i> - and <i>dl</i> -Serine. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2945-2953.	1.1	74
4210	Periodic and Molecular Modeling Study of Donor-Acceptor Interactions in (dbbpy)Pt(tdt)·TENF and [Pt(dbbpy)(tdt)] ₂ ·TENF. <i>Organometallics</i> , 2010, 29, 795-800.	1.1	12
4211	Visible Light Sensitization of TiO ₂ Surfaces with Alq3 Complexes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 1317-1325.	1.5	37
4212	Revealing the Magnetostructural Dynamics of [2Fe-2S] Ferredoxins from Reduced-Dimensionality Analysis of Antiferromagnetic Exchange Coupling Fluctuations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11612-11619.	1.2	14
4213	"Carbene Radicals" in Co ^{II} (por)-Catalyzed Olefin Cyclopropanation. <i>Journal of the American Chemical Society</i> , 2010, 132, 10891-10902.	6.6	301
4214	Bisamidate and Mixed Amine/Amidate Ni ₂ S ₂ Complexes as Models for Nickel-Containing Acetyl Coenzyme A Synthase and Superoxide Dismutase: An Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2010, 49, 5393-5406.	1.9	64
4215	Asymmetry and Electronegativity in the Electron Capture Activation of the Se-Se Bond: $\dot{I}f^*(Se\dot{S}e)$ vs $\dot{I}f^*(Se\dot{S}X)$. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3102-3112.	2.3	15
4216	Cooperative Cation Migrations upon CO Addition in CuI- and Alkali-Exchanged Faujasite: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 17802-17811.	1.5	25
4217	Role of Heme Distortion on Oxygen Affinity in Heme Proteins: The Protoglobin Case. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8536-8543.	1.2	49
4218	Synthesis and Characterization of the Ground and Excited States of Tripodal-like Oligothieryl-imidazoles. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4964-4972.	1.2	27
4219	Anion Photoelectron Spectroscopy of C ₃ N ⁺ and C ₅ N ⁺ . <i>Journal of Physical Chemistry A</i> , 2010, 114, 3215-3220.	1.1	32
4220	Description of Mg ²⁺ Release from Forsterite Using Ab Initio Methods. <i>Journal of Physical Chemistry C</i> , 2010, 114, 5417-5428.	1.5	20

#	ARTICLE	IF	CITATIONS
4221	Synthesis and characterization of heterooligonuclear ruthenium complexes with tri(phenanthroline)hexaazatriphenylene ligands. <i>Journal of Coordination Chemistry</i> , 2010, 63, 2727-2742.	0.8	10
4222	Carbamate Transport in Carbamoyl Phosphate Synthetase: A Theoretical and Experimental Investigation. <i>Journal of the American Chemical Society</i> , 2010, 132, 3870-3878.	6.6	13
4223	Kinetics of Hydrogen Abstraction Reactions of Butene Isomers by OH Radical. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12088-12098.	1.1	56
4224	Quantum-Chemical Study of the Effect of Triethylaluminum on the Chain-End Structure, Reactivity, and Microtacticity of Poly(<i>N,N</i> -dimethylacrylamide) with Lithium Counterion in Nonpolar Solvents. <i>Macromolecules</i> , 2010, 43, 6337-6342.	2.2	1
4225	Neutral <i>cis</i> -Alkyl Olefin Rhodium(I) Complexes: Models of Intermediates in Late Transition Metal Olefin Polymerization with Surprising Structure. <i>Organometallics</i> , 2010, 29, 5496-5503.	1.1	21
4226	One-Electron Oxidation of Individual DNA Bases and DNA Base Stacks. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1860-1867.	1.1	13
4227	Modeling the Structural and Electronic Properties of an Optically Active Regioregular Polythiophene. <i>Journal of Physical Chemistry C</i> , 2010, 114, 11074-11080.	1.5	11
4228	Ab Initio Chemical Kinetics for SiH_3 Reactions with $\text{Si}_x\text{H}_{2x+2}$ ($x = 1-4$). <i>Journal of Physical Chemistry A</i> , 2010, 114, 13353-13361.	1.1	8
4229	Synthesis and Structure of Intermediates in Copper-Catalyzed Alkylation of Diphenylphosphine. <i>Inorganic Chemistry</i> , 2010, 49, 7650-7662.	1.9	56
4230	Theoretical Investigation on the Effect of Protonation on the Absorption and Emission Spectra of Two Amine-Group-Bearing, Red σ -Push π -Pull σ -Emitters, 4-Dimethylamino-4'-nitrostilbene and 4-(dicyanomethylene)-2-methyl-6-(dimethylamino) styryl-4H-pyran, by DFT and TDDFT Calculations. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5580-5587.	1.1	42
4231	Transition Metal Intervention for a Classic Reaction: Assessing the Feasibility of Nickel(0)-Promoted [1,3] Sigmatropic Shifts of Bicyclo[3.2.0]hept-2-enes. <i>Organometallics</i> , 2010, 29, 3541-3545.	1.1	18
4232	Valence Bond/Broken Symmetry Analysis of the Exchange Coupling Constant in Copper(II) Dimers. Ferromagnetic Contribution Exalted through Combined Ligand Topology and (Singlet) Covalent-Ionic Mixing. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6149-6156.	1.1	32
4233	Configurationally Labile Enantioenriched Lithiated 3-Arylprop-2-enyl Carbamates: Joint Experimental and Quantum Chemical Investigations on the Equilibrium of Epimers. <i>Journal of Organic Chemistry</i> , 2010, 75, 5716-5720.	1.7	9
4234	Oxo- and Hydroxomanganese(IV) Adducts: A Comparative Spectroscopic and Computational Study. <i>Inorganic Chemistry</i> , 2010, 49, 7530-7535.	1.9	43
4235	Water-Assisted Dehalogenation of Thionyl Chloride in the Presence of Water Molecules. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4123-4130.	1.1	15
4236	Crossed-Beam Investigation of $\text{O}(^3\text{P}) + \text{C}_2\text{H}_5\text{C}(\text{OH})_2 + \text{C}_2\text{H}_4$. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4891-4895.	1.1	7
4237	Differentiating Mechanistic Possibilities for the Thermal, Intramolecular [2 + 2] Cycloaddition of Allene π -Ynes. <i>Journal of the American Chemical Society</i> , 2010, 132, 11952-11966.	6.6	94
4238	Understanding the Dynamics Behind the Photoisomerization of a Light-Driven Fluorene Molecular Rotary Motor. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5058-5067.	1.1	96

#	ARTICLE	IF	CITATIONS
4239	Remarkable Reactions and Intermediates in Titanocene(IV) Chemistry: Migratory Insertion Reactions of 2,2-Disubstituted-1-alkenes, Intramolecular 1,5- σ -Bond Metathesis via η^5 -Agostic Interactions, and a Rare Example of a η^2 -Agostic Alkyltitanocene Complex. <i>Journal of the American Chemical Society</i> , 2010, 132, 13357-13370.	6.6	30
4240	Formation of Aminyl Radicals on Electron Attachment to AZT: Abstraction from the Sugar Phosphate Backbone versus One-Electron Oxidation of Guanine. <i>Journal of Physical Chemistry B</i> , 2010, 114, 9289-9299.	1.2	19
4241	Caged Chalcogens: Theoretical Studies on a Tetracoordinated Oxonium Dication and Its Higher Homologues. <i>Organic Letters</i> , 2010, 12, 772-775.	2.4	13
4242	Auxiliary Density Matrix Methods for Hartree-Fock Exchange Calculations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2348-2364.	2.3	438
4243	Spectroscopic and Computational Studies of a Series of High-Spin Ni(II) Thiolate Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 6535-6544.	1.9	9
4244	Fluxionality of $[(Ph)_3P]_3M(X)$ ($M = Rh, Ir$). The Red and Orange Forms of $[(Ph)_3P]_3Ir(Cl)$. Which Phosphine Dissociates Faster from Wilkinson's Catalyst?. <i>Journal of the American Chemical Society</i> , 2010, 132, 12013-12026.	6.6	50
4245	Nonlinear Optical Switching Properties in the Furfurylfulgide Aberchrome 540's Dihydrobenzofuran Derivative Pair of Photochromic Materials. <i>Journal of Physical Chemistry A</i> , 2010, 114, 673-679.	1.1	15
4246	Systematic Investigation of CD Spectra of Aryl Benzyl Sulfoxides Interpreted by Means of TDDFT Calculations. <i>Journal of Organic Chemistry</i> , 2010, 75, 1143-1154.	1.7	43
4247	Comprehensive Density Functional Theory Study on the Mechanism of Activation of the Nonapeptide Hormone Oxytocin by Metal Ions. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1417-1423.	1.2	14
4248	Reaction Intermediates during the Dehydrogenation of Metal Borohydrides: A Cluster Perspective. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16849-16854.	1.5	32
4249	Assessing the Performance of Density Functional Theory for the Electronic Structure of Metal-Salens: The M06 Suite of Functionals and the d^{10} -Metals. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11714-11718.	1.1	35
4250	A Series of Peroxomanganese(III) Complexes Supported by Tetradentate Aminopyridyl Ligands: Detailed Spectroscopic and Computational Studies. <i>Journal of the American Chemical Society</i> , 2010, 132, 2821-2831.	6.6	64
4251	Quantum Refinement of Protein Structures: Implementation and Application to the Red Fluorescent Protein DsRed.M1. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15413-15423.	1.2	28
4252	Contact Geometry Symmetry Dependence of Field Effect Gating in Single-Molecule Transistors. <i>Journal of the American Chemical Society</i> , 2010, 132, 2914-2918.	6.6	12
4253	Holo-Ni(II)HpNikR Is an Asymmetric Tetramer Containing Two Different Nickel-Binding Sites. <i>Journal of the American Chemical Society</i> , 2010, 132, 14447-14456.	6.6	36
4254	Quantum Mechanical and Quantum Mechanical/Molecular Mechanical Studies of the Iron's Dioxygen Intermediates and Proton Transfer in Superoxide Reductase. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2896-2909.	2.3	19
4255	Redox Mechanism of Glycosidic Bond Hydrolysis Catalyzed by 6-Phospho- α -glucosidase: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11196-11206.	1.2	30
4256	Formation of Beyerene, Kaurene, Trachylobane, and Atiserene Diterpenes by Rearrangements That Avoid Secondary Carbocations. <i>Journal of the American Chemical Society</i> , 2010, 132, 5375-5386.	6.6	77

#	ARTICLE	IF	CITATIONS
4257	The Role of Exact Exchange in the Description of $\text{Cu}^{2+}(\text{H}_2\text{O})_6$ Complexes by Means of DFT Methods. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10857-10863.	1.1	43
4258	Continuous Localized Orbital Corrections to Density Functional Theory: B3LYP-CLOC. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3647-3663.	2.3	9
4259	Desymmetrizations Forming Tetrasubstituted Olefins Using Enantioselective Olefin Metathesis. <i>Organic Letters</i> , 2010, 12, 2032-2035.	2.4	63
4260	Dehydroindigo, the Forgotten Indigo and Its Contribution to the Color of Maya Blue. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1699-1708.	1.1	58
4261	Use of Metallopeptide Based Mimics Demonstrates That the Metalloprotein Nitrile Hydratase Requires Two Oxidized Cysteines for Catalytic Activity. <i>Inorganic Chemistry</i> , 2010, 49, 9064-9077.	1.9	19
4262	Shielding Constants and Chemical Shifts in DFT: Influence of Optimized Effective Potential and Coulomb-Attenuation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7179-7186.	1.1	18
4263	Sulfur-Based Redox Reactions in $\text{Mo}_3\text{S}_7^{4+}$ and $\text{Mo}_3\text{S}_4^{4+}$ Clusters Bearing Halide and 1,2-Dithiolene Ligands: a Mass Spectrometric and Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2010, 49, 8045-8055.	1.9	11
4264	Insights into Photoinduced Electron Transfer between $[\text{Ru}(\text{bpy})_3]^{2+}$ and $[\text{S}_2\text{O}_8]^{2-}$ in Water: Computational and Experimental Studies. <i>Journal of Physical Chemistry A</i> , 2010, 114, 73-80.	1.1	51
4265	Computational Study of Methane C-H Activation by First-Row Late Transition Metal $\text{L}^{\text{M}}\text{E}$ (M: Fe, Co, Ni) Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 2038-2046.	1.9	56
4266	A Diffusion Monte Carlo Study of the O-H Bond Dissociation of Phenol. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9832-9835.	1.1	15
4267	Structural Determinants for the Stereoselective Hydrolysis of Chiral Substrates by Phosphotriesterase. <i>Biochemistry</i> , 2010, 49, 7988-7997.	1.2	25
4268	Theoretical Studies on the Mechanisms and Dynamics of OH Radicals with $\text{CH}_2\text{FCF}_2\text{OCHF}_2$ and $\text{CH}_2\text{FOCH}_2\text{F}$. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9057-9068.	1.1	19
4269	The Quest for Tetracoordinated Halonium Ions: A Theoretical Investigation. <i>Organic Letters</i> , 2010, 12, 4844-4847.	2.4	5
4270	Theoretical Investigations on the Reaction of Monosubstituted Tertiary-Benzylamine Selenols with Hydrogen Peroxide. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10706-10711.	1.1	16
4271	Electronic structure and ionicity of actinide oxides from first principles. <i>Physical Review B</i> , 2010, 81, .	1.1	123
4272	Time-Resolved Resonance Raman Studies on Proton-Induced Electron-Transfer Reaction from Triplet Excited State of 2-Methoxynaphthalene to Decafluorobenzophenone. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12447-12451.	1.1	2
4273	A Topological Study of the Decomposition of 6,7,8-Trioxabicyclo[3.2.2]nonane Induced by Fe(II): Modeling the Artemisinin Reaction with Heme. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1163-1173.	1.2	5
4274	Alumina as a Simultaneous Support and Co Catalyst: Cationic Hafnium Complex Evidenced by Experimental and DFT Analyses. <i>Journal of Physical Chemistry C</i> , 2010, 114, 18516-18528.	1.5	23

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4275	Multiple Low-Lying States for Compound I of P450 _{cam} and Chloroperoxidase Revealed from Multireference Ab Initio QM/MM Calculations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 940-953.	2.3	66
4276	Conformational Preferences of Proline Analogues with a Fused Benzene Ring. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11761-11770.	1.2	15
4277	Role of π -Conjugation in Influencing the Magnetic Interactions in Dinitrenes: A Broken-Symmetry Approach. <i>Journal of Physical Chemistry A</i> , 2010, 114, 93-96.	1.1	6
4278	Investigating the Anharmonicity of Lattice Vibrations in Water-Containing Molecular Crystals through the Terahertz Spectroscopy of α -Serine Monohydrate. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9570-9578.	1.1	55
4279	Toward the Design of Ferromagnetic Molecular Complexes: Magnetostructural Correlations in Ferromagnetic Triply Bridged Dinuclear Cu(II) Compounds Containing Carboxylato and Hydroxo Bridges. <i>Inorganic Chemistry</i> , 2010, 49, 285-294.	1.9	30
4280	A Theoretical Investigation of the Photophysical Consequences of Major Plant Light-Harvesting Complex Aggregation within the Photosynthetic Membrane. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15244-15253.	1.2	17
4281	Dinuclear Dicyclopentadienyl Titanium Complexes with Bridging Cyclopentadienylsiloxo Ligands. <i>Organometallics</i> , 2010, 29, 642-655.	1.1	6
4282	Synthesis of Gold Phosphido Complexes Derived from Bis(secondary) Phosphines. Structure of Tetrameric $[\text{Au}(\text{MesP}(\text{CH}_2)_2)_3\text{PMe}_2\text{Au}]_4$. <i>Inorganic Chemistry</i> , 2010, 49, 3950-3957.	1.9	21
4283	What Is the Preferred Structure of the Meisenheimer [†] Wheland Complex Between <i>trans</i> -Triaminobenzene and 4,6-Dinitrobenzofuroxan?. <i>Journal of Organic Chemistry</i> , 2010, 75, 3761-3765.	1.7	14
4284	Large Changes in Electronic Structures of Ru ₂ ⁶⁺ Species Caused by the Variations of the Bite Angle of Guanidinate Ligands: Tuning Magnetic Behavior. <i>Inorganic Chemistry</i> , 2010, 49, 3051-3056.	1.9	19
4285	Reinvestigation of the Reaction of Ethylene and Singlet Oxygen by the Approximate Spin Projection Method. Comparison with Multireference Coupled-Cluster Calculations. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7967-7974.	1.1	44
4286	SEIRA and SERS Effects in Cyclopentabithiophenethiol-Capped Gold Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12900-12904.	1.5	11
4287	Formation Enthalpies of Ions: Routine Prediction Using Atom Equivalentents. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2126-2139.	2.3	4
4288	Kinetics and Thermodynamics of the Monomer [†] Dimer Equilibria of Dialkoxydibutylstannanes. <i>Organometallics</i> , 2010, 29, 6384-6392.	1.1	16
4289	An Assessment of Density Functional Methods for Potential Energy Curves of Nonbonded Interactions: The XYG3 and B97-D Approximations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 727-734.	2.3	91
4290	Ab Initio Molecular Dynamics Study of the Reaction between Th ⁺ and H ₂ O ⁺ . <i>Journal of Physical Chemistry A</i> , 2010, 114, 8613-8617.	1.1	24
4291	A System-Dependent Density-Based Dispersion Correction. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1990-2001.	2.3	133
4292	How an Enzyme Might Accelerate an Intramolecular Diels [†] Alder Reaction: Theozymes for the Formation of Salvileucalin B. <i>Organic Letters</i> , 2010, 12, 1164-1167.	2.4	19

#	ARTICLE	IF	CITATIONS
4293	Reaction Pathway of Methylenation of Carbonyl Compounds with Bis(iodozincio)methane. <i>Journal of the American Chemical Society</i> , 2010, 132, 17452-17458.	6.6	34
4294	Trends in R ^α X Bond Dissociation Energies (R ^α = Me, Et, i-Pr, t-Bu, X = H, Me, Cl, OH). <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1462-1469.	2.3	39
4295	Ab Initio Studies of Structural and Vibrational Properties of Protonated Water Cluster H ₇ O ₃ ⁺ and Its Deuterium Isotopologues: An Application of Driven Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2525-2535.	2.3	32
4296	Computational Insights into the Mechanism of Porphobilinogen Synthase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 16860-16870.	1.2	17
4297	Molecular Dynamics Studies on Native, Loop-Contracted, and Metal Ion-Substituted Azurins. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8474-8486.	1.2	15
4298	Theoretical and Raman Spectroscopic Studies of Phenolic Lignin Model Monomers. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8009-8021.	1.2	86
4299	Self-assembly of supramolecular Ni(II) and Cu(II) metalmacrocylic compounds with tetraazamacrocyclic ligand into a gelatin-immobilized matrix. <i>Journal of Coordination Chemistry</i> , 2010, 63, 4309-4318.	0.8	23
4300	Synthesis and X-ray Structure of a Diamagnetic Oxo-Bridged Trifluoromethyl ^α Chromium(V) Complex: Structural and Computational Comparisons between CF ₃ and CH ₃ Ligands in Two Different Oxidation States of Chromium. <i>Organometallics</i> , 2010, 29, 3672-3675.	1.1	10
4301	Multi-Length Scale Morphology of Poly(ethylene oxide)-Based Sulfonate Ionomers with Alkali Cations at Room Temperature. <i>Macromolecules</i> , 2010, 43, 4223-4229.	2.2	76
4302	Germynes: Structures, Electron Affinities, and Singlet ^α Triplet Gaps of the Conventional XGeCY ₃ (X = H, F, Cl, Br, and I; Y = F and Cl) Species and the Unexpected Cyclic XGeCY ₃ (Y = Br and I) Systems. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13198-13212.	1.1	6
4303	Electronic Structural Comparison of the Reactions of Dioxygen and Alkenes with Nitrogen-Chelated Palladium(0). <i>Inorganic Chemistry</i> , 2010, 49, 8200-8207.	1.9	23
4304	Cascade [1,3]-Sigmatropic Rearrangements of Ketene <i>α</i> O _α , <i>α</i> O _α -Acetals: Kinetic and DFT Level Mechanistic Studies. <i>Journal of Organic Chemistry</i> , 2010, 75, 1898-1910.	1.7	6
4305	Transport of Metallic Ions through Polyaniline-Containing Composite Membranes. <i>Journal of Chemical & Engineering Data</i> , 2010, 55, 4801-4807.	1.0	17
4306	Favored Reaction Mechanism of Calcium-Dependent Phospholipase A ₂ . Insights from Density Functional Exploration. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11584-11593.	1.2	5
4307	Poly(2-thiophen-3-yl-malonic acid), a Polythiophene with Two Carboxylic Acids Per Repeating Unit. <i>Journal of Physical Chemistry B</i> , 2010, 114, 6281-6290.	1.2	33
4308	Tuned Range-Separated Hybrids in Density Functional Theory. <i>Annual Review of Physical Chemistry</i> , 2010, 61, 85-109.	4.8	661
4309	Electronic Transition Energies: A Study of the Performance of a Large Range of Single Reference Density Functional and Wave Function Methods on Valence and Rydberg States Compared to Experiment. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 370-383.	2.3	202
4310	Multireference Character of 1,3-Dipolar Cycloaddition of Ozone with Ethylene and Acrylonitrile. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12116-12123.	1.1	24

#	ARTICLE	IF	CITATIONS
4311	Stabilization and Structure Calculations for Noncovalent Interactions in Extended Molecular Systems Based on Wave Function and Density Functional Theories. <i>Chemical Reviews</i> , 2010, 110, 5023-5063.	23.0	697
4312	Thermochemical benchmarking of hydrocarbon bond separation reaction energies: Jacob's ladder is not reversed!. <i>Molecular Physics</i> , 2010, 108, 2655-2666.	0.8	53
4313	Single Electron Transfer and S_N2 Reactions: The Importance of Ionization Potential of Nucleophiles. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 602-606.	2.3	20
4314	How Well Can Kohn-Sham DFT Describe the $HO_2 + O_3$ Reaction?. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2751-2761.	2.3	21
4315	A first principles study of the oxidation energetics and kinetics of realgar. <i>Geochimica Et Cosmochimica Acta</i> , 2010, 74, 4266-4284.	1.6	24
4316	First-principles study of Ge isotope fractionation during adsorption onto Fe(III)-oxyhydroxide surfaces. <i>Chemical Geology</i> , 2010, 278, 15-22.	1.4	46
4317	Computer-aided structure analysis of an epimerized dehydroepiandrosterone derivative and its biological effect in a model of reactive gliosis. <i>Steroids</i> , 2010, 75, 265-271.	0.8	2
4318	Unravelling the stereoselectivity in 6-exo-trig radical cyclization of $\hat{1},\hat{1}^2$ -unsaturated ester-tethered sugars. A tale of two stereocenters. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 1619.	1.5	0
4319	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2071-2085.	2.3	383
4320	X-ray Diffraction, Solution Structure, and Computational Studies on Derivatives of (3- <i>sec</i> -Butyl-2,3-dihydro-1 <i>H</i> -isoquinolin-4-ylidene)acetic Acid: Compounds with Activity as Calpain Inhibitors. <i>Journal of Organic Chemistry</i> , 2010, 75, 342-352.	1.7	5
4321	Density functional approximations for charge transfer excitations with intermediate spatial overlap. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12697.	1.3	101
4322	Tuning the Optoelectronic Properties of Vinylene-Linked Donor-Acceptor Copolymers for Organic Photovoltaics. <i>Macromolecules</i> , 2010, 43, 6685-6698.	2.2	86
4323	Analysis of the Reactivities of Protein C-H Bonds to H Atom Abstraction by OH Radical. <i>Journal of the American Chemical Society</i> , 2010, 132, 16450-16459.	6.6	38
4324	The carbocation continuum in terpene biosynthesis—where are the secondary cations?. <i>Chemical Society Reviews</i> , 2010, 39, 2847.	18.7	147
4325	Theoretical Study of the Gas-Phase Reactions of Iodine Atoms ($I_2P_{3/2}$) with H_2 , H_2O , HI, and OH. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9270-9288.	1.1	32
4326	Describing Anions by Density Functional Theory: Fractional Electron Affinity. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2726-2735.	2.3	104
4327	Quantum Chemical Study on UV-vis Spectra of Microhydrated Iodine Dimer Radical Anion. <i>Journal of Physical Chemistry A</i> , 2010, 114, 721-724.	1.1	10
4328	Dissecting a Dyotropic Rearrangement. <i>Journal of Organic Chemistry</i> , 2010, 75, 1693-1700.	1.7	23

#	ARTICLE	IF	CITATIONS
4329	Effect of the Substituent and Hydrogen Bond on the Geometry and Electronic Properties of OH and O ⁺ Groups in para-Substituted Phenol and Phenolate Derivatives. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10885-10890.	1.1	14
4330	Protonated [4n] and [4n+2] Octaphyrins Choose Their Macrocyclic Aromatic Topology. <i>Journal of the American Chemical Society</i> , 2010, 132, 3105-3114.	6.6	116
4331	The Influence of Local Electric Fields on Photoinduced Absorption in Dye-Sensitized Solar Cells. <i>Journal of the American Chemical Society</i> , 2010, 132, 9096-9101.	6.6	196
4332	Hybrid functional study of proper and improper multiferroics. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5405.	1.3	147
4333	Self-Assembly of Structurally Persistent Micelles Is Controlled by Specific-Ion Effects and Hydrophobic Guests. <i>Langmuir</i> , 2010, 26, 10460-10466.	1.6	22
4334	Electronic structure of LiCoO_2 films: A combined photoemission spectroscopy and density functional theory study. <i>Physical Review B</i> , 2010, 82, .	1.1	60
4335	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8016.	1.3	126
4336	Molecular Design of Organic Dye toward Retardation of Charge Recombination at Semiconductor/Dye/Electrolyte Interface: Introduction of Twisted π -Linker. <i>Journal of Physical Chemistry C</i> , 2010, 114, 17920-17925.	1.5	73
4337	Mechanistic and Kinetic Study of $\text{CH}_2\text{O} + \text{O}_3$ Reaction. <i>Journal of Physical Chemistry A</i> , 2010, 114, 3516-3522.	1.1	28
4338	Structure and stability of the heteroannulated [8n+10]circulenes: A quantum-chemical study. <i>Pure and Applied Chemistry</i> , 2010, 82, 1011-1024.	0.9	20
4339	Generalized Koopmans density functional calculations reveal the deep acceptor state of ZnO . <i>Physical Review B</i> , 2010, 81, .	1.1	135
4340	Single-particle and quasiparticle interpretation of Kohn-Sham and generalized Kohn-Sham eigenvalues for hybrid functionals. <i>Physical Review B</i> , 2010, 82, .	1.1	58
4341	The resolution of the identity approximation for calculations of spin-spin contribution to zero-field splitting parameters. <i>Journal of Chemical Physics</i> , 2010, 132, 144111.	1.2	49
4342	Electric Field Gradients Calculated from Two-Component Hybrid Density Functional Theory Including Spin-Orbit Coupling. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2669-2686.	2.3	47
4343	Orientational order of a ferroelectric liquid crystal with small layer contraction. <i>Physical Review E</i> , 2010, 82, 031702.	0.8	11
4344	Direct Observation of the Gas Phase Reaction of the Cyclohexyl Radical with Dioxygen Using a Distonic Radical Ion Approach. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1446-1456.	1.1	41
4345	Unidirectional Photoisomerization of Styrylpyridine for Switching the Magnetic Behavior of an Iron(II) Complex: A MLCT Pathway in Crystalline Solids. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21715-21722.	1.5	42
4346	Photodissolution of Ferrihydrite in the Presence of Oxalic Acid: An In Situ ATR-FTIR/DFT Study. <i>Langmuir</i> , 2010, 26, 16246-16253.	1.6	53

#	ARTICLE	IF	CITATIONS
4347	Examining the Planarity of Poly(3,4-ethylenedioxythiophene): Consideration of Self-Rigidification, Electronic, and Geometric Effects. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1023-1028.	1.1	38
4348	From Poly(3,4-ethylenedioxythiophene) to Poly(3,4-phenylenedioxythiophene): Impact of the Substitution of the Ethylene Bridge by the Phenyl Ring on the Molecular Properties. <i>Journal of Physical Chemistry B</i> , 2010, 114, 3494-3499.	1.2	10
4349	Relativistic Density Functional Theory. Challenges and Advances in Computational Chemistry and Physics, 2010, , 191-214.	0.6	13
4350	Experimental and theoretical study on activation of the C-H bond in pyridine by [Mm] (M = Cu, Ag, Au,) Tj ETO _q] 1 0.784314 rg	1.3	5
4351	Mechanisms of the Au- and Pt-Catalyzed Intramolecular Acetylenic Schmidt Reactions: A DFT Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 7842-7854.	1.7	57
4352	Comparison of ruthenium(ii) and cyclometalated iridium(iii) azacrown ether phenanthroline hybrids for the detection of metal cations by electrochemiluminescence. <i>Dalton Transactions</i> , 2010, 39, 5130.	1.6	65
4353	Vibronic coupling in indole: I. Theoretical description of the 1La-1Lb interaction and the electronic spectrum. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4968.	1.3	84
4354	(Py) ₂ Co(CH ₂) ₂ SiMe ₃) ₂ As an Easily Accessible Source of α -CoR ₂ . <i>Organometallics</i> , 2010, 29, 1897-1908.	1.1	47
4355	Frontiers in electronic structure theory. <i>Journal of Chemical Physics</i> , 2010, 132, 110902.	1.2	147
4356	[14]Annulene: Cis/Trans Isomerization via Two-Twist and Nondegenerate Planar Bond Shifting and M π Conformational Minima. <i>Organic Letters</i> , 2010, 12, 972-975.	2.4	9
4357	The [13]Annulene Cation Is a Stable M π Annulene Cation. <i>Organic Letters</i> , 2010, 12, 1708-1711.	2.4	24
4358	Assignment of UV-vis Spectrum of (3,3 α)-Diindolylmethane, a <i>Leishmania donovani</i> Topoisomerase IB Inhibitor and a Candidate DNA Minor Groove Binder. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7121-7126.	1.1	7
4359	The role of hyperconjugative π -aromaticity in the enhanced acidity of methyl-, silyl and germlycyclopentadienes. <i>Molecular Physics</i> , 2010, 108, 2467-2476.	0.8	7
4360	Theoretical Study of the Addition of OH Radicals to <i>trans</i> -(3,7-dimethylocta-2,6-dien-1-ol), 6-Methyl-5-hepten-2-one, and 6-Hydroxy-4-methyl-4-hexenal. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5468-5477.	1.1	4
4361	Thermopower of correlated semiconductors: Application to FeAs	1.1	80
4362	Defect physics of CuGaS	1.2	62
4363	Hybrid density functional calculations of redox potentials and formation energies of transition metal compounds. <i>Physical Review B</i> , 2010, 82, .	1.1	298
4364	Quantum chemical topology study on the electronic structure of <i>cis</i> - and <i>trans</i> -FONO. <i>Journal of Chemical Physics</i> , 2010, 133, 034304.	1.2	13

#	ARTICLE	IF	CITATIONS
4365	Chemical Distinction by Nuclear Spin Optical Rotation. <i>Physical Review Letters</i> , 2010, 105, 153001.	2.9	39
4366	Applications of the Cluster Method for Biological Systems. <i>Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems</i> , 2010, 1, 71-150.	0.6	1
4367	Epoxidation of Alkenes with Hydrogen Peroxide Catalyzed by Selenium-Containing Dinuclear Peroxotungstate and Kinetic, Spectroscopic, and Theoretical Investigation of the Mechanism. <i>Inorganic Chemistry</i> , 2010, 49, 2471-2478.	1.9	59
4368	Role of 1,2-Dimethoxyethane in the Transformation from Ethylene Polymerization to Trimerization Using Chromium Tris(2-ethylhexanoate)-Based Catalyst System: A DFT Study. <i>Organometallics</i> , 2010, 29, 1588-1602.	1.1	53
4369	Improved Description of the Structure of Molecular and Layered Crystals: Ab Initio DFT Calculations with van der Waals Corrections. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11814-11824.	1.1	895
4370	Solvatochromic and Ionochromic Effects of Iron(II)bis(1,10-phenanthroline)dicyano: a Theoretical Study. <i>Inorganic Chemistry</i> , 2010, 49, 1634-1646.	1.9	26
4371	¹⁴ N NQR, ¹ H NMR and DFT/QTAIM study of hydrogen bonding and polymorphism in selected solid 1,3,4-thiadiazole derivatives. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13007.	1.3	18
4372	Reduction of Hydrogen Peroxide by Glutathione Peroxidase Mimics: Reaction Mechanism and Energetics. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1996-2000.	1.1	29
4373	Ethanolysis of N-substituted norbornane epoxyimides: Discovery of diverse pathways depending on substituent's character. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 2142-57.	1.5	9
4374	Periodic DFT Study of Radical Species on Crystalline Silica Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16430-16438.	1.5	27
4375	Polythiophenes Containing In-Chain Cobaltabisdicarbollide Centers. <i>ACS Applied Materials & Interfaces</i> , 2010, 2, 691-702.	4.0	29
4376	Synthesis and structural characterisation of germanium(ii) halide complexes with neutral N-donor ligands. <i>Dalton Transactions</i> , 2010, 39, 847-856.	1.6	55
4377	Orbital-dependent Representation of Correlation Energy Functional. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 455-466.	1.4	2
4378	Ferromagnetically Coupled Cobalt-Benzene-Cobalt: The Smallest Molecular Spin Filter with Unprecedented Spin Injection Coefficient. <i>Journal of the American Chemical Society</i> , 2010, 132, 15334-15339.	6.6	37
4379	Enzymatic Ring-Opening Mechanism of Verdoheme by the Heme Oxygenase: A Combined X-ray Crystallography and QM/MM Study. <i>Journal of the American Chemical Society</i> , 2010, 132, 12960-12970.	6.6	38
4380	DFT Study of Paramagnetic Adducts of Tris-(8-hydroxyquinoline)aluminum (III). <i>Journal of Physical Chemistry A</i> , 2010, 114, 12759-12763.	1.1	10
4381	Validation of Density Functional Methods for the Calculation of Small Gold Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10297-10308.	1.1	43
4382	Benzothiazole-Based Fluorophores of Donor-Acceptor-Donor Type Displaying High Two-Photon Absorption. <i>Journal of Organic Chemistry</i> , 2010, 75, 3053-3068.	1.7	135

#	ARTICLE	IF	CITATIONS
4383	Geometric structures and electron affinities of chlorine-doped silicon clusters. <i>Molecular Physics</i> , 2010, 108, 1919-1927.	0.8	0
4384	A tangled web of interconnecting pathways to amorphadiene and the amorphene sesquiterpenes. <i>Chemical Science</i> , 2010, 1, 609.	3.7	32
4385	Prototropic equilibria in DNA containing one-electron oxidized GC: intra-duplex vs. duplex to solvent deprotonation. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5353.	1.3	54
4386	Application of high level wavefunction methods in quantum mechanics/molecular mechanics hybrid schemes. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5041.	1.3	18
4387	Hydrogen bonding in electronically excited states: a comparison between formic acid dimer and its mono-substituted thioderivatives. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13037.	1.3	8
4388	Adsorption-induced structural changes of gold cations from two- to three-dimensions. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3038.	1.3	20
4389	Reactivity of the $\text{AlF}_3(100)$ surface: defects, fluorine mobility and catalysis of the CCl_2F_2 dismutation reaction. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6124.	1.3	10
4390	The thiocyanate anion as a polydentate halogen bond acceptor. <i>CrystEngComm</i> , 2010, 12, 558-566.	1.3	67
4391	Excited state polarizabilities of methanol clusters. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2929.	1.3	14
4392	A combined crossed-beam and ab initio study of the atom radical reaction dynamics of $\text{O}(^3\text{P}) + \text{C}_2\text{H}_5^+$. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7098.	1.3	12
4393	Are cyclopentadienylberyllium, magnesium and calcium hydrides carbon or metal acids in the gas phase?. <i>Dalton Transactions</i> , 2010, 39, 4593.	1.6	11
4394	Muon spin spectroscopy of the discotic liquid crystal HAT6. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9900.	1.3	8
4395	Slow photoelectron velocity-map imaging of the C_nH^{n-} ($n = 5-9$) anions. <i>Chemical Science</i> , 2010, 1, 192.	3.7	16
4396	Self-Assembly of a Designed Amyloid Peptide Containing the Functional Thienylalanine Unit. <i>Journal of Physical Chemistry B</i> , 2010, 114, 10674-10683.	1.2	24
4397	Interpretation of the Ultrafast Photoinduced Processes in Pentacene Thin Films. <i>Journal of the American Chemical Society</i> , 2010, 132, 3431-3439.	6.6	59
4398	Tetrahedral Tungsten Oxide Clusters W_4O_n ($n = 10-13$): Structural Evolution and Chemical Bonding. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1964-1972.	1.1	23
4399	Testing High-Level QM/MM Methods for Modeling Enzyme Reactions: Acetyl-CoA Deprotonation in Citrate Synthase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11303-11314.	1.2	61
4400	Structures and Phase Transitions in $(\text{MoO}_2)_2\text{P}_2\text{O}_7$. <i>Inorganic Chemistry</i> , 2010, 49, 2290-2301.	1.9	27

#	ARTICLE	IF	CITATIONS
4401	Infrared Spectra of a Species of Potential Prebiotic and Astrochemical Interest: Cyanoethenethiol (NC \equiv CH \cdot CH \cdot SH). <i>Journal of Physical Chemistry A</i> , 2010, 114, 9583-9588.	1.1	8
4402	Conformational Profile of a Proline \sim Arginine Hybrid. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1781-1789.	2.5	4
4403	Effects of spin-orbit coupling and strong correlation on the paramagnetic insulating state in plutonium dioxides. <i>Physical Review B</i> , 2010, 82, .	1.1	38
4404	Configurations and conformations of glycosyl sulfoxides. <i>Canadian Journal of Chemistry</i> , 2010, 88, 1154-1174.	0.6	7
4405	Inversion of the shuttlecock shaped metal phthalocyanines MPc (M = Ge, Sn, Pb) \hat{a} €”a density functional study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6179.	1.3	26
4406	Mass-spectrometric and computational study of tryptophan radicals (Trp + H) \dot{E} ™ produced by collisional electron transfer to protonated tryptophan in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13434.	1.3	17
4407	Carbon and proton shielding tensors in methyl halides. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2679.	1.3	52
4408	The influence of the relative position of the thiophene and pyrrole rings in donor \hat{a} €”acceptor thienylpyrrolyl-benzothiazole derivatives. A photophysical and theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9719.	1.3	31
4409	DNA interaction with Ru(ii) and Ru(ii)/Cu(ii) complexes containing azamacrocycle and dppz residues. A thermodynamic, kinetic and theoretical study.. <i>Dalton Transactions</i> , 2010, 39, 9838.	1.6	14
4410	Radical allylations by reaction of azides with allylindium dichloride. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 3444.	1.5	10
4411	Electron capture activation of the disulfide bond. The role of the asymmetry and electronegativity. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1042-1050.	1.3	17
4412	Zn(ii)-coordination and fluorescence studies of a new polyazamacrocycle incorporating 1H-pyrazole and naphthalene units. <i>Dalton Transactions</i> , 2010, 39, 7741.	1.6	7
4413	Unexpected dissociation energetics of the Na ⁺ counterion from GC motifs in DNA hole-migration. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13099.	1.3	3
4414	Nanocapsule with pump for methane storage. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 9863.	1.3	3
4415	On the multiple B \hat{a} €”N bonding in boron compounds using the topological analysis of electron localization function (ELF). <i>New Journal of Chemistry</i> , 2011, 35, 89-96.	1.4	40
4416	New electron correlation theories for transition metal chemistry. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6750.	1.3	120
4417	On multiferroicity of TTF-CA molecular crystal. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 144-148.	1.3	15
4418	Band gap engineering of double-cation-impurity-doped anatase-titania for visible-light photocatalysts: a hybrid density functional theory approach. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13698.	1.3	39

#	ARTICLE	IF	CITATIONS
4419	Structure, morphology and interface properties of ultrathin SnTTBPP(OH) ₂ -films adsorbed on Ag(100). <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 9839.	1.3	4
4420	Theoretical studies on the mechanism and stereoselectivity of Rh(Phebox)-catalyzed asymmetric reductive aldol reaction. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5845.	1.5	26
4421	Relativistic effects on group-12 metal nuclear shieldings. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 21016.	1.3	35
4422	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. <i>International Reviews in Physical Chemistry</i> , 2011, 30, 115-160.	0.9	116
4423	Why BLUF photoreceptors with roseoflavinocofactors lose their biological functionality. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14775.	1.3	16
4424	Pincer ligands with an all-phosphorus donor set: subtle differences between rhodium and palladium. <i>Dalton Transactions</i> , 2011, 40, 8822.	1.6	52
4425	Kohn-Sham Density Functional Theory Electronic Structure Calculations with Linearly Scaling Computational Time and Memory Usage. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 340-350.	2.3	88
4426	Performance of Conventional and Range-Separated Hybrid Density Functionals in Calculations of Electronic Circular Dichroism Spectra of Transition Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14677-14686.	1.1	26
4427	The Taxadiene-Forming Carbocation Cascade. <i>Journal of the American Chemical Society</i> , 2011, 133, 18249-18256.	6.6	49
4428	Thickness, Surface Morphology, and Optical Properties of Porphyrin Multilayer Thin Films Assembled on Si(100) Using Copper(I)-Catalyzed Azide-Alkyne Cycloaddition. <i>Langmuir</i> , 2011, 27, 4613-4622.	1.6	38
4429	Moving up and down the Titanium Oxidation State in Ziegler-Natta Catalysis. <i>Macromolecules</i> , 2011, 44, 778-783.	2.2	91
4430	Synthesis, Optical Characterization, and Electrochemical Properties of Isomeric Tetraphenylbenzodifurans Containing Electron Acceptor Groups. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4157-4168.	1.1	17
4431	Phosphorus and phosphorus-nitrogen doped carbon nanotubes for ultrasensitive and selective molecular detection. <i>Nanoscale</i> , 2011, 3, 1008-1013.	2.8	102
4432	A computational study of cycloaddition reactions of d8 metal tetroxide (Iron, Ruthenium, Osmium) complexes with C ₆₀ . <i>Dalton Transactions</i> , 2011, 40, 4122.	1.6	2
4433	Controlling dynamic stereoisomerism in transition-metal folded baskets. <i>Chemical Science</i> , 2011, 2, 752.	3.7	14
4434	Accounting for non-optimal interactions in molecular recognition: a study of ion complexes using a QM/MM model with a dipole-polarisable MM region. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19401.	1.3	5
4435	Addition of Hydrocarbons to Si(100) in Extra-Mild Conditions: A Novel Mechanism Valid for Single and Multiple C-C Bonds. <i>Journal of Physical Chemistry C</i> , 2011, 115, 19210-19215.	1.5	5
4436	Thermal C-H Bond Activation of Benzene, Toluene, and Methane with Cationic [M(X)(bipy)] ⁺ (M = Ni, Pd, Tj) ETQq _{1,1} 0.784314 rB ₄₆ (K	1.1	46

#	ARTICLE	IF	CITATIONS
4437	Potential Energy Curve for Ring-Opening Reactions: Comparison Between Broken-Symmetry and Multireference Coupled Cluster Methods. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5625-5631.	1.1	17
4438	Reaction-Induced Magnetic Transition in Mn ²⁺ Dimers. <i>Journal of Physical Chemistry A</i> , 2011, 115, 549-555.	1.1	11
4439	How and Why Do Transition Dipole Moment Orientations Depend on Conformer Structure?. <i>Journal of Physical Chemistry A</i> , 2011, 115, 9612-9619.	1.1	18
4440	First-principles computational studies of the torsional potential energy surface of the <i>cis</i> -butyl radical. <i>Canadian Journal of Chemistry</i> , 2011, 89, 1469-1476.	0.6	3
4441	Theoretical study on the gas phase reaction of acrylonitrile with a hydroxyl radical. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16585.	1.3	25
4442	Evaluation of potential reaction mechanisms leading to the formation of coniferyl alcohol β -linkages in lignin: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20974.	1.3	14
4443	Antiferromagnetic interactions in the quarter-filled organic conductor (EDO-TTF)2PF6. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 12328.	1.3	9
4444	Nitrosyl induces phosphorous-acid dissociation in ruthenium(ii). <i>Dalton Transactions</i> , 2011, 40, 12917.	1.6	9
4445	⁹⁵ Mo nuclear magnetic resonance parameters of molybdenum hexacarbonyl from density functional theory: appraisal of computational and geometrical parameters. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19471.	1.3	12
4446	Photophysical and quantum chemical study on a J-aggregate forming perylene bisimide monomer. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 17649.	1.3	42
4447	On the PES for the interaction of an H atom with an H chemisorbate on a graphenic platelet. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 17579.	1.3	13
4448	O–O Bond activation in H ₂ O ₂ and (CH ₃) ₃ C-OOH mediated by [Ni(cyclam)(CH ₃ CN) ₂](ClO ₄) ₂ : Different mechanisms to form the same Ni(III) product?. <i>Dalton Transactions</i> , 2011, 40, 6868.	1.6	15
4449	Spectroscopic and computational characterization of Cu ^{II} -OOR (R = H or cumyl) complexes bearing a Me ₆ -tren ligand. <i>Dalton Transactions</i> , 2011, 40, 2234.	1.6	39
4450	A gas-phase crossed-beam study of OH produced in the radical–radical reaction of O(3P) with iso-propyl radical (CH ₃) ₂ CH. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 8122.	1.3	8
4451	Ionization potentials of adenine along the internal conversion pathways. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15492.	1.3	28
4452	A critical theoretical study on the two-photon absorption properties of some selective triaryl borane-1-naphthylphenyl amine based charge transfer molecules. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 9285.	1.3	24
4453	Stability trends and tautomerization of chalcocyclopentadienes. The role of aromaticity. <i>New Journal of Chemistry</i> , 2011, 35, 2713.	1.4	4
4454	Intramolecular hydrogen bonding controls 1,3-N,S- vs. 1,5-S,S ²⁻ -coordination in NiII complexes of N-thiophosphorylated thioureas RNHC(S)NHP(S)(OiPr) ₂ . <i>Dalton Transactions</i> , 2011, 40, 3142.	1.6	30

#	ARTICLE	IF	CITATIONS
4455	Nuclear spin relaxation due to chemical shift anisotropy of gas-phase ^{129}Xe . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13704.	1.3	17
4456	An organocatalytic approach to enantiomerically enriched $\hat{\pm}$ -arylcyclohexenones and cyclohexanones. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 8253.	1.5	17
4457	The effect of the position of methyl substituents on photophysical and photochemical properties of $[\text{Ru}(\text{x}, \text{x}\text{-dmb})(\text{CN})_4]^{2+}$ complexes: experimental confirmation of the theoretical predictions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16033.	1.3	4
4458	Silene equivalents through the rhodium-catalysed reactions of $\hat{\pm}$ -hypersilyl diazoesters: a computational and experimental study. <i>Chemical Science</i> , 2011, 2, 2367.	3.7	9
4459	The benzene+OH potential energy surface: intermediates and transition states. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2214-2221.	1.3	28
4460	Theoretical investigation of the complexation of crown ethers and crown ethers of fulleropyrrolidine with $(\text{CH}_3)_x\text{NH}^+4$, $x = 0-4$. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 954-965.	1.3	10
4461	Theoretical studies on the structural and magnetic property of arginase active site. <i>Supramolecular Chemistry</i> , 2011, 23, 22-28.	1.5	3
4462	Solvent-Assisted Naked Eye Sensing of Hg^{2+} by a Chemoreceptor Derived from Diazocoupling of Sulfathiazole with Diethyl Malonate. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2011, 186, 1820-1834.	0.8	3
4463	Dissociation of H_2NCH_2 Dication in a Strong Laser Field. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8375-8379.	1.1	6
4464	Quantitative Assessment of Force Fields on Both Low-Energy Conformational Basins and Transition-State Regions of the $(\hat{\pm})$ Space. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 402-419.	2.3	10
4465	A Stable Aminothioketyl Radical in the Gas Phase. <i>Journal of the American Chemical Society</i> , 2011, 133, 10290-10301.	6.6	1
4466	Thermal Stability of Endohedral First-Row Transition-Metal $\text{TM}@ZnSi$ Structures, $i = 12, 16$. <i>Journal of Physical Chemistry C</i> , 2011, 115, 7829-7835.	1.5	7
4467	Effective Fragment Potential Study of the Influence of Hydration on the Vibrational Spectrum of Glucose. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12373-12379.	1.1	10
4468	Theoretical Study of the Stability and Electronic Structure of $\text{Al}(\text{BH}_4)_n$ and $\text{Al}(\text{BF}_4)_n$ and Their Hyperhalogen Behavior. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10237-10243.	1.1	69
4469	The Need for Enzymatic Steering in Abietic Acid Biosynthesis: Gas-Phase Chemical Dynamics Simulations of Carbocation Rearrangements on a Bifurcating Potential Energy Surface. <i>Journal of the American Chemical Society</i> , 2011, 133, 8335-8343.	6.6	69
4470	Xanthene-Modified and Hangman Iron Corroles. <i>Inorganic Chemistry</i> , 2011, 50, 1368-1377.	1.9	52
4471	First-principles study of electronic and structural properties of CuO . <i>Physical Review B</i> , 2011, 84, .	1.1	106
4472	Experimental, SOPPA(CCSD), and DFT Analysis of Substituent Effects on NMR JCF Coupling Constants in Fluorobenzene Derivatives. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1272-1279.	1.1	32

#	ARTICLE	IF	CITATIONS
4473	Environmental Effects on the Lignin Model Monomer, Vanillyl Alcohol, Studied by Raman Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2011, 115, 11470-11480.	1.2	20
4474	Kinetic Modeling of the Free-Radical Process during the Initiated Thermal Cracking of Normal Alkanes with 1-Nitropropane as an Initiator. <i>Industrial & Engineering Chemistry Research</i> , 2011, 50, 9054-9062.	1.8	18
4475	MAPping the Chiral Inversion and Structural Transformation of a Metal-Tripeptide Complex Having Ni-Superoxide Dismutase Activity. <i>Inorganic Chemistry</i> , 2011, 50, 2479-2487.	1.9	28
4476	Wavelet Transform for Spectroscopic Analysis: Application to Diols in Water. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1109-1118.	2.3	23
4477	Computational Study of Cycloaddition Reactions of 16-Electron $d^{8} ML_{4}$ Complexes with C_{60} . <i>Journal of Physical Chemistry A</i> , 2011, 115, 7664-7672.	1.1	7
4478	Helimeric Porphyrinoids: Stereostructure and Chiral Resolution of meso-Tetraarylmorpholinochlorins. <i>Journal of the American Chemical Society</i> , 2011, 133, 8740-8752.	6.6	58
4479	Localization of Electronic Excitations in Conjugated Polymers Studied by DFT. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 566-571.	2.1	96
4480	Coarse-Grained Molecular Dynamics Simulations of the Sphere to Rod Transition in Surfactant Micelles. <i>Langmuir</i> , 2011, 27, 6628-6638.	1.6	130
4481	Electronic structure of cation-codoped TiO ₂ for visible-light photocatalyst applications from hybrid density functional theory calculations. <i>Applied Physics Letters</i> , 2011, 98, 142103.	1.5	38
4482	Substituent Effect on the Acid-Promoted Hydrolysis of 2-Aryloxazolin-5-one: Normal vs Reverse. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4995-5004.	1.1	6
4483	Synthesis, Structures, and Properties of the Phosphonium-1-indenylide (PHIN) Ligands 1-C ₉ H ₆ PPh ₃ , 1-C ₉ H ₆ PMePh ₂ , and 1-C ₉ H ₆ PMe ₂ Ph and of the Corresponding Ruthenium(II) Complexes [Ru(η^5 -C ₅ H ₅)(η^5 -PHIN)]PF ₆ . <i>Organometallics</i> , 2011, 30, 6098-6107.	1.1	11
4484	Computational Insight into the Electronic Structure and Absorption Spectra of Lithium Complexes of N-Confused Tetraphenylporphyrin. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11749-11760.	1.1	17
4485	Introduction of a New Theory for the Calculation of Magnetic Coupling Based on Spin-Flip Constricted Variational Density Functional Theory. Application to Trinuclear Copper Complexes which Model the Native Intermediate in Multicopper Oxidases. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1858-1866.	2.3	41
4486	Charge-Transfer-Like $\hat{\rho}^{\dagger}\hat{\rho}$ Excitations in Time-Dependent Density Functional Theory: A Conundrum and Its Solution. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2408-2415.	2.3	221
4487	Density Functional Theory Studies on Ice Nanotubes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12841-12851.	1.1	9
4488	Selectivity and Mechanism of Hydrogen Atom Transfer by an Isolable Imidoiron(III) Complex. <i>Journal of the American Chemical Society</i> , 2011, 133, 9796-9811.	6.6	128
4489	Stability of Hydrocarbons of the Polyhedrane Family: Convergence of ab Initio Calculations and Corresponding Assessment of DFT Main Approximations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2761-2765.	2.3	3
4490	Electron Localization Function Study on Intramolecular Electron Transfer in the QTTFQ and DBTTFI Radical Anions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13513-13522.	1.1	12

#	ARTICLE	IF	CITATIONS
4491	Ligand Topology Effect on the Reactivity of a Mononuclear Nonheme Iron(IV)-Oxo Complex in Oxygenation Reactions. <i>Journal of the American Chemical Society</i> , 2011, 133, 11876-11879.	6.6	94
4492	Stereoselectivities and Regioselectivities of (4 + 3) Cycloadditions Between Allenamide-Derived Chiral Oxazolidinone-Stabilized Oxyallyls and Furans: Experiment and Theory. <i>Journal of the American Chemical Society</i> , 2011, 133, 14443-14451.	6.6	55
4493	Detailed Investigation of the OH Radical Quenching by Natural Antioxidant Caffeic Acid Studied by Quantum Mechanical Models. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4218-4233.	2.3	100
4494	First-Principle Calculations on the Microscopic $\langle \sup{57} \rangle$ Fe Electric-Field-Gradient Tensor of Ferrous Chloride Tetrahydrate: A Prototypical MÅ†ssbauer Species. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10655-10663.	1.1	1
4495	Bond Length Alternation of Conjugated Oligomers: Wave Function and DFT Benchmarks. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 369-376.	2.3	131
4496	DFT Study on the Radical Anions Formed by Primaquine and Its Derivatives. <i>Chemical Research in Toxicology</i> , 2011, 24, 1476-1485.	1.7	12
4497	Application of London-Type Dispersion Corrections in Solid-State Density Functional Theory for Predicting the Temperature-Dependence of Crystal Structures and Terahertz Spectra. <i>Crystal Growth and Design</i> , 2011, 11, 2006-2010.	1.4	19
4498	Effect of Nitrogen Adsorption on the Mid-Infrared Spectrum of Water Clusters. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6218-6225.	1.1	23
4499	Iron(0) Promotes Aza Cyclization of an Elusive Ferrocenylketene. <i>Organometallics</i> , 2011, 30, 4830-4837.	1.1	13
4500	Nonorthogonality Problem and Effective Electronic Coupling Calculation: Application to Charge Transfer in i€-Stacks Relevant to Biochemistry and Molecular Electronics. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1712-1725.	2.3	52
4501	Theoretical Investigation for the Cycle Reaction of $N_{\langle \sub{2} \rangle}O$ ($x_{\langle \sup{1} \rangle} \hat{\langle \sup{+} \rangle}$) with CO ($\langle \sup{1} \rangle \hat{\langle \sup{+} \rangle}$) Catalyzed by $IrO_{\langle \sub{\langle i \rangle n \langle /i \rangle} \rangle}$ ($\langle i \rangle n \langle /i \rangle = 1$). <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 100</i> <i>Journal of Physical Chemistry A</i> , 2011, 115, 11023-11032.	1.1	13
4502	“NHâ€” Termination of the Si(111) Surface by Wet Chemistry. <i>Journal of the American Chemical Society</i> , 2011, 133, 20769-20777.	6.6	44
4503	Effect of Hubbard U on the construction of low-energy Hamiltonians for $LaMnO_3$ via maximally localized Wannier functions. <i>Physical Review B</i> , 2011, 84, .	1.1	13
4504	Comparison of Multistandard and TMS-Standard Calculated NMR Shifts for Coniferyl Alcohol and Application of the Multistandard Method to Lignin Dimers. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1958-1970.	1.2	39
4505	TD-CI Simulation of the Electronic Optical Response of Molecules in Intense Fields II: Comparison of DFT Functionals and EOM-CCSD. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11832-11840.	1.1	42
4506	How Is a Co-Methyl Intermediate Formed in the Reaction of Cobalamin-Dependent Methionine Synthase? Theoretical Evidence for a Two-Step Methyl Cation Transfer Mechanism. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4066-4077.	1.2	44
4507	Development of a Polarizable Force Field for Molecular Dynamics Simulations of Poly (Ethylene) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 100</i>	2.3	39
4508	Density Functional Reactivity Theory Characterizes Charge Separation Propensity in Proton-Coupled Electron Transfer Reactions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4738-4742.	1.1	25

#	ARTICLE	IF	CITATIONS
4509	Effect of Substituted Groups on the Electronic Circular Dichroism of Aldols: A Combined Experimental and Time-Dependent DFT Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 972-981.	1.5	5
4510	Thermal Decomposition of 2-Butanol as a Potential Nonfossil Fuel: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2837-2846.	1.1	36
4511	Theoretical Study of Magnetic Properties of Oxovanadium(IV) Complex Self-Assemblies with Tetradentate Schiff Base Ligands. <i>Journal of Physical Chemistry B</i> , 2011, 115, 8465-8473.	1.2	8
4512	Surface Structure and Reactivity of Rhodium Oxide. <i>Journal of Physical Chemistry C</i> , 2011, 115, 11036-11044.	1.5	33
4513	First-Principles Study of Rectification in Bis-2-(5-ethynylthienyl)ethyne Molecular Junctions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 9033-9042.	1.1	16
4514	pB ₂ Intermediate of the Photoactive Yellow Protein: Structure and Excitation Energies. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2097-2106.	1.2	8
4515	Comparison of Intermolecular Interaction Energies from SAPT and DFT Including Empirical Dispersion Contributions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11321-11330.	1.1	48
4516	Electronically Coupled Tetrathiafulvalene Electrophores across a Non-innocent Acetylidate-Ruthenium Bridge. <i>Organometallics</i> , 2011, 30, 3570-3578.	1.1	42
4517	Quinoxaline-Embedded Polyacenoquinone Esters: Synthesis, Electronic Properties, and Crystal Structure. <i>Organic Letters</i> , 2011, 13, 4588-4591.	2.4	11
4518	Theoretical Studies of Electron Transport in Thiophene Dimer: Effects of Substituent Group and Heteroatom. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4535-4546.	1.1	30
4519	Oscillator Strengths in ONIOM Excited State Calculations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 180-187.	2.3	10
4520	Changes in the Electronic Structures of a Single Sheet of Sashlike Polydiacetylene Atomic Sash upon Structural Transformations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 9518-9525.	1.5	4
4521	Structure, Conformation, Stereodynamics, and Absolute Configuration of the Atropisomers of Fluorenylidene Derivatives. <i>Journal of Organic Chemistry</i> , 2011, 76, 1487-1490.	1.7	2
4522	Simulating the Reactivity of a Disordered Surface of the TiCN Thin Film. <i>Journal of Physical Chemistry C</i> , 2011, 115, 15432-15439.	1.5	2
4523	Theoretical Study of the Decomposition of BCl ₃ Induced by a H Radical. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4786-4797.	1.1	8
4524	Synthesis, Characterization, Interionic Structure, and Self-Aggregation Tendency of Zirconaziridinium Salts Bearing Long Alkyl Chains. <i>Organometallics</i> , 2011, 30, 100-114.	1.1	45
4525	Investigation of Uranyl Nitrate Ion Pairs Complexed with Amide Ligands Using Electrospray Ionization Ion Trap Mass Spectrometry and Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3497-3508.	1.1	15
4526	Structural and Electronic Properties of Poly[N-(2-cyanoalkyl)pyrrole]s Bearing Small Alkyl Groups. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2882-2889.	1.2	7

#	ARTICLE	IF	CITATIONS
4527	Accurate Calculation of Chemical Shifts in Highly Dynamic H ₂ @C ₆₀ through an Integrated Quantum Mechanics/Molecular Dynamics Scheme. Organic Letters, 2011, 13, 2528-2531.	2.4	11

4528

#	ARTICLE	IF	CITATIONS
4545	Comparative Study on the Performance of Hybrid DFT Functionals in Highly Correlated Oxides: The Case of CeO ₂ and Ce ₂ O ₃ . Journal of Chemical Theory and Computation, 2011, 7, 56-65.	2.3	125
4546	First-principles optical response of semiconductors and oxide materials. Physical Review B, 2011, 83, .	1.1	51
4547	Aryl C-H Amination by Diruthenium Nitrides in the Solid State and in Solution at Room Temperature: Experimental and Computational Study of the Reaction Mechanism. Journal of the American Chemical Society, 2011, 133, 13138-13150.	6.6	61
4548	Photophysical properties of Kuratowski-type coordination compounds [MIIZn4Cl4(Me2bta)6] (MII = Zn) Tj ETQq1 1.6 0.784314 rgBT /Q	1.6	29
4549	Excited-State Dynamics in 6-Thioguanosine from the Femtosecond to Microsecond Time Scale. Journal of Physical Chemistry B, 2011, 115, 3263-3270.	1.2	97
4550	Structure and properties of oxygen centers in CaF ₂ crystals from <i>ab initio</i> embedded cluster calculations. Physical Review B, 2011, 84, .	1.1	22
4551	Understanding Optoelectronic Properties of Cyano-Terminated Oligothiophenes in the Context of Intramolecular Charge Transfer. Journal of Physical Chemistry B, 2011, 115, 10573-10585.	1.2	23
4552	Electron-density descriptors as predictors in quantitative structure-activity/property relationships and drug design. Future Medicinal Chemistry, 2011, 3, 969-994.	1.1	53
4553	Hole Transport in Triphenylamine Based OLED Devices: From Theoretical Modeling to Properties Prediction. Journal of Physical Chemistry A, 2011, 115, 14519-14525.	1.1	154
4554	Transition States and Energetics of Nucleophilic Additions of Thiols to Substituted α,β -Unsaturated Ketones: Substituent Effects Involve Enone Stabilization, Product Branching, and Solvation. Journal of Organic Chemistry, 2011, 76, 5074-5081.	1.7	84
4555	Electronic levels and electrical response of periodic molecular structures from plane-wave orbital-dependent calculations. Physical Review B, 2011, 84, .	1.1	19
4556	The excited state dipole moments of betaine pyridinium investigated by an innovative solvatochromic analysis and TDDFT calculations. Physical Chemistry Chemical Physics, 2011, 13, 13185.	1.3	27
4557	TD-DFT Vibronic Couplings in Anthraquinones: From Basis Set and Functional Benchmarks to Applications for Industrial Dyes. Journal of Chemical Theory and Computation, 2011, 7, 1882-1892.	2.3	113
4559	Electronic structure and bonding properties of cobalt oxide in the spinel structure. Physical Review B, 2011, 83, .	1.1	258
4560	Density functional theory calculations of dynamic first hyperpolarizabilities for organic molecules in organic solvent: Comparison to experiment. Journal of Chemical Physics, 2011, 135, 134104.	1.2	37
4561	Band-edge problem in the theoretical determination of defect energy levels: The O vacancy in ZnO as a benchmark case. Physical Review B, 2011, 84, .	1.1	143
4562	Double-hybrid density-functional theory made rigorous. Journal of Chemical Physics, 2011, 134, 064113.	1.2	165
4563	Highly enantioselective cascade synthesis of spiropyrazolones. Organic and Biomolecular Chemistry, 2011, 9, 6519.	1.5	104

#	ARTICLE	IF	CITATIONS
4564	Accurate Band Gaps for Semiconductors from Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 212-217.	2.1	444
4565	Mechanistic Studies of Ethylene Hydrophenylation Catalyzed by Bipyridyl Pt(II) Complexes. <i>Journal of the American Chemical Society</i> , 2011, 133, 19131-19152.	6.6	76
4567	Oscillator Strength: How Does TDDFT Compare to EOM-CCSD?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 456-466.	2.3	123
4568	A computational investigation on singlet and triplet exciton couplings in acene molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18615.	1.3	44
4569	Systematic Study of the Performance of Density Functional Theory Methods for Prediction of Energies and Geometries of Organoselenium Compounds. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4827-4831.	1.1	29
4570	Electronic Structure of Aromatic Monomolecular Films: The Effect of Molecular Spacers and Interfacial Dipoles. <i>Journal of Physical Chemistry C</i> , 2011, 115, 22422-22428.	1.5	21
4571	The Harvard Clean Energy Project: Large-Scale Computational Screening and Design of Organic Photovoltaics on the World Community Grid. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2241-2251.	2.1	470
4572	A DFT study on the mechanism of gold(III)-catalyzed synthesis of highly substituted furans via [3, 3]-sigmatropic rearrangements and/or [1, 2]-acyloxy migration based on propargyl ketones. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 2760.	1.5	30
4573	Ruthenium(II) complexes: structure, DNA-binding, photocleavage, antioxidant activity, and theoretical studies. <i>Journal of Coordination Chemistry</i> , 2011, 64, 3792-3807.	0.8	19
4574	Benzothiazoles with Tunable Electron-Withdrawing Strength and Reverse Polarity: A Route to Triphenylamine-Based Chromophores with Enhanced Two-Photon Absorption. <i>Journal of Organic Chemistry</i> , 2011, 76, 8726-8736.	1.7	138
4575	Quantum Mechanical Investigation of the Effect of Catalyst Fluorination in the Intermolecular Asymmetric Stetter Reaction. <i>Journal of the American Chemical Society</i> , 2011, 133, 11249-11254.	6.6	89
4576	Stoichiometric and Oxygen-Rich M_2O_n and M_2O_n ($M = Nb, Ta; n = 5-7$) Clusters: Molecular Models for Oxygen Radicals, Diradicals, and Superoxides. <i>Journal of the American Chemical Society</i> , 2011, 133, 3085-3094.	6.6	49
4577	A Parameter-Free Density Functional That Works for Noncovalent Interactions. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 983-989.	2.1	134
4578	Nitrogenase Structure and Function Relationships by Density Functional Theory. <i>Methods in Molecular Biology</i> , 2011, 766, 267-291.	0.4	5
4580	Gas-Phase Acidity Studies of Dual Hydrogen-Bonding Organic Silanols and Organocatalysts. <i>Journal of Organic Chemistry</i> , 2011, 76, 7186-7194.	1.7	47
4581	Exceptionally Strong Magnetism in the $R_2M_2O_{10}$ perovskites ($R = Nb, Ta; n = 5-7$) Clusters. <i>Journal of the American Chemical Society</i> , 2011, 133, 11249-11254.	1.1	42
4582	Solvation Structure and Dynamics of Ni^{2+} (aq) from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2937-2946.	2.3	11
4583	Modeling the Tetraphenylalanine-PEG Hybrid Amphiphile: From DFT Calculations on the Peptide to Molecular Dynamics Simulations on the Conjugate. <i>Journal of Physical Chemistry B</i> , 2011, 115, 8937-8946.	1.2	23

#	ARTICLE	IF	CITATIONS
4584	A Sulfonium Cation Intermediate in the Mechanism of Methionine Sulfoxide Reductase B: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9202-9212.	1.2	12
4586	A comparative analysis of the UV/Vis absorption spectra of nitrobenzaldehydes. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 4269.	1.3	17
4587	Electronic structure and reactivity of a biradical cluster: Sc ₃ O ₆ ³⁻ . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10084.	1.3	32
4588	The Î±-Amino Group of the Threonine Substrate as The General Base During tRNA Aminoacylation: A New Version of Substrate-Assisted Catalysis Predicted by Hybrid DFT. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13050-13060.	1.1	18
4589	Does DFT-D estimate accurate energies for the binding of ligands to metal complexes?. <i>Dalton Transactions</i> , 2011, 40, 11176.	1.6	81
4590	First Principles Calculations of Atomic Nickel Redox Potentials and Dimerization Free Energies: A Study of Metal Nanoparticle Growth. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 485-495.	2.3	33
4591	Mechanistic Analysis of Muraymycin Analogues: A Guide to the Design of MraY Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 8421-8439.	2.9	79
4592	Theoretical Studies of Homogeneous Catalysts Mimicking Nitrogenase. <i>Molecules</i> , 2011, 16, 442-465.	1.7	24
4593	First-principles GW calculations for fullerenes, porphyrins, phthalocyanine, and other molecules of interest for organic photovoltaic applications. <i>Physical Review B</i> , 2011, 83, .	1.1	362
4594	Quantum mechanics/molecular mechanics methods can be more accurate than full quantum mechanics in systems involving dispersion correlations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10520.	1.3	18
4595	Toward Reliable DFT Investigations of Mn-Porphyrins through CASPT2/DFT Comparison. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3532-3539.	2.3	25
4596	The chemistry of acetone at extreme conditions by density functional molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2011, 134, 064502.	1.2	0
4597	First-principles study of boron oxygen hole centers in crystals: Electronic structures and nuclear hyperfine and quadrupole parameters. <i>Physical Review B</i> , 2011, 84, .	1.1	17
4598	Three Dimensional Models of Cu ²⁺ -A ¹⁶ Complexes from Computational Approaches. <i>Journal of the American Chemical Society</i> , 2011, 133, 15008-15014.	6.6	61
4599	Dinuclear Zn(II) Complex Catalyzed Phosphodiester Cleavage Proceeds via a Concerted Mechanism: A Density Functional Theory Study. <i>Journal of the American Chemical Society</i> , 2011, 133, 2904-2915.	6.6	55
4600	Computational Studies on Structural and Excited-State Properties of Modified Chlorophyll with Various Axial Ligands. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12298-12306.	1.1	14
4601	Revisiting the Effects of Sequence and Structure on the Hydrogen Bonding and Î€-Stacking Interactions in Nucleic Acids. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12800-12808.	1.1	15
4602	Crystal field and magnetic structure of UO ₂ . <i>Physical Review B</i> , 2011, 83, .	1.1	49

#	ARTICLE	IF	CITATIONS
4603	Efficient and accurate local single reference correlation methods for high-spin open-shell molecules using pair natural orbitals. <i>Journal of Chemical Physics</i> , 2011, 135, 214102.	1.2	165
4604	The fate of optical excitations in small polyhedral ZnS clusters: A theoretical study of the excitation and localization of electrons in Zn ₄ S ₄ and Zn ₆ S ₆ . <i>Journal of Chemical Physics</i> , 2011, 134, 064511.	1.2	18
4605	Topological Study of the Late Steps of the Artemisinin Decomposition Process: Modeling the Outcome of the Experimentally Obtained Products. <i>Journal of Physical Chemistry B</i> , 2011, 115, 333-346.	1.2	2
4606	Comparative density functional theory and post-Hartree-Fock (CCSD, CASSCF) studies on the electronic structure of halogen nitrites ClONO and BrONO using quantum chemical topology. <i>Journal of Chemical Physics</i> , 2011, 135, 094303.	1.2	3
4607	Hybrid density functional theory description of N- and C-doping of NiO. <i>Journal of Chemical Physics</i> , 2011, 134, 224703.	1.2	34
4608	Luminescent bichromophoric spiroindolones – synthesis and electronic properties. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 6196.	1.5	40
4609	Scalar Relativistic Computations of Nuclear Magnetic Shielding and $\langle i \rangle g \langle i \rangle$ -Shifts with the Zeroth-Order Regular Approximation and Range-Separated Hybrid Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3278-3292.	2.3	42
4610	Interplay of Correlation and Relativistic Effects in Correlated Calculations on Transition-Metal Complexes: The (Cu ₂ O) ²⁺ Core Revisited. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1511-1523.	2.3	104
4611	Atmospheric Chemistry of Two Biodiesel Model Compounds: Methyl Propionate and Ethyl Acetate. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8906-8919.	1.1	35
4612	Pyrene-based organic dyes with thiophene containing π -linkers for dye-sensitized solar cells: optical, electrochemical and theoretical investigations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 17210.	1.3	59
4613	Thermal Generation and Structures of the Unsaturated Doubly Bridged Complex [Mo ₂ Cp ₂ Cl ₂ (η^4 -SMe) ₂] and Its Quadruply Bridged Isomer [Mo ₂ Cp ₂ (η^4 -Cl) ₂ (η^4 -SMe) ₂]. <i>Organometallics</i> , 2011, 30, 649-652.	1.1	5
4614	Reaction Mechanism for the Thermal Decomposition of BCl ₃ /CH ₄ /H ₂ Gas Mixtures. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11579-11588.	1.1	9
4615	Oxidation mechanism of diethyl ether: a complex process for a simple molecule. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14636.	1.3	73
4616	Density Functional Calculation of the Structure and Electronic Properties of Cu _n O _n ($n = 1 \sim 8$) Clusters. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2087-2095.	1.1	39
4617	Estimation of Mayr Electrophilicity with a Quantitative Structure–Property Relationship Approach Using Empirical and DFT Descriptors. <i>Journal of Organic Chemistry</i> , 2011, 76, 9312-9319.	1.7	21
4618	Local structure of Mn ⁴⁺ and Fe ³⁺ spin probes in layered LiAlO ₂ oxide by modelling of zero-field splitting parameters. <i>Dalton Transactions</i> , 2011, 40, 9106.	1.6	10
4619	A Synthesis of Pseudoconhydrine and Its Epimer via Hydroformylation and Dihydroxylation. <i>Journal of Organic Chemistry</i> , 2011, 76, 6844-6848.	1.7	34
4620	Theoretical Studies on Molecular and Structures of Mono- and Binuclear Chromium Carbazole Derivatives for Optoelectronics. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14495-14501.	1.1	17

#	ARTICLE	IF	CITATIONS
4621	HSE hybrid functional within the FLAPW method and its application to GdN. <i>Physical Review B</i> , 2011, 84, .	1.1	34
4622	A Density Functional Theory for Studying Ionization Processes in Water Clusters. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5735-5744.	1.1	51
4623	Thermodynamic modelling of nanomorphologies of hematite and goethite. <i>Journal of Materials Chemistry</i> , 2011, 21, 11566.	6.7	114
4624	Structural and Optical Properties of Isolated Noble Metal- γ -Glutathione Complexes: Insight into the Chemistry of Liganded Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2011, 115, 24549-24554.	1.5	34
4625	Double-Hybrid Density Functionals Provide a Balanced Description of Excited π and σ States in Polycyclic Aromatic Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3272-3277.	2.3	84
4626	Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. <i>Physical Review B</i> , 2011, 83, .	1.1	159
4627	Spectroscopic and Computational Studies of Glutathionylcobalamin: Nature of Co-S Bonding and Comparison to Co-C Bonding in Coenzyme B ₁₂ . <i>Inorganic Chemistry</i> , 2011, 50, 8755-8766.	1.9	25
4628	Ruthenium Complexes of Thiaporphyrin and Dithiaporphyrin. <i>Inorganic Chemistry</i> , 2011, 50, 11947-11957.	1.9	20
4629	Cooperative Double Deprotonation of Bis(2-picoly)amine Leading to Unexpected Bimetallic Mixed Valence (M ^I , M ^{II}) Rhodium and Iridium Complexes. <i>Inorganic Chemistry</i> , 2011, 50, 7524-7534.	1.9	25
4630	Redox-Active Ligands and Organic Radical Chemistry. <i>Inorganic Chemistry</i> , 2011, 50, 9879-9887.	1.9	115
4631	Evaluation of the Nonlinear Optical Properties for Annulenes with Hückel and Möbius Topologies. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3935-3943.	2.3	86
4632	Excited States and Absorption Spectra of UF ₆ : A RASPT2 Theoretical Study with Spin-Orbit Coupling. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3223-3231.	2.3	19
4633	Ditantalum Dinitrogen Complex: Reaction of H ₂ Molecule with End-on-Bridged μ -[Ta ^{IV}] ₂ (μ -N) and Bis(μ -nitrido) [Ta ^V] ₂ (μ -N) ₂ Complexes. <i>Inorganic Chemistry</i> , 2011, 50, 9481-9490.	1.9	23
4634	Geometric and Electronic Structures of Peroxomanganese(III) Complexes Supported by Pentadentate Amino-Pyridine and -imidazole Ligands. <i>Inorganic Chemistry</i> , 2011, 50, 10190-10203.	1.9	43
4635	BH ₃ -Promoted Stereoselective β -Lithiation of <i>N</i> -Alkyl-2-phenylaziridines. <i>Journal of Organic Chemistry</i> , 2011, 76, 2291-2295.	1.7	22
4636	Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advanced ab initio methods. <i>Physical Review B</i> , 2011, 84, .	1.1	66
4637	Hemibonding of Hydroxyl Radical and Halide Anion in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14620-14628.	1.1	30
4638	Calculations on the Structure and Spectral Properties of Cytochrome <i>c</i> ₅₅₁ Using DFT and ONIOM Methods. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2866-2876.	1.1	7

#	ARTICLE	IF	CITATIONS
4640	A DFT comparison of the neutral and cationic Heck pathways. Dalton Transactions, 2011, 40, 11308.	1.6	36
4641	NMR Shielding Constants in PH ₃ , Absolute Shielding Scale, and the Nuclear Magnetic Moment of ³¹ P. Journal of Physical Chemistry A, 2011, 115, 10617-10623.	1.1	39
4642	Density functional investigation of Fe clusters (n = 6) with Cr substitutions: UB3LYP/LanL2DZ calculation. Computational Materials Science, 2011, 50, 982-990.	1.4	11
4643	A high-throughput infrastructure for density functional theory calculations. Computational Materials Science, 2011, 50, 2295-2310.	1.4	787
4644	B3LYP investigation of response properties of alkali halides on external static electric fields. Computational Materials Science, 2011, 50, 2628-2635.	1.4	6
4645	Complexation of alkali metal cations by conformationally rigid, stereoisomeric calix[4]arene crown ethers: A density functional theory study. Computational and Theoretical Chemistry, 2011, 967, 235-242.	1.1	8
4646	Theoretical investigation on the reaction of N ₂ O and CO catalyzed by PtO ⁺ . Computational and Theoretical Chemistry, 2011, 968, 31-38.	1.1	6
4647	A theoretical study of the structure and electron density of the peptide bond. Computational and Theoretical Chemistry, 2011, 969, 76-82.	1.1	11
4648	A natural bond orbital analysis of hydrocarbon radicals. Computational and Theoretical Chemistry, 2011, 970, 73-78.	1.1	4
4649	Tautomerism in polyguanide. Computational and Theoretical Chemistry, 2011, 971, 58-64.	1.1	13
4650	Theoretical studies on the reactions of thymine with six methylating agents. Computational and Theoretical Chemistry, 2011, 972, 25-31.	1.1	1
4651	Theoretical views on the cycle reaction of N ₂ O (1 ⁺)+NH ₃ (1A ₁)+O ₂ catalyzed by Fe ⁺ and utilizing the energy span model to study its kinetic information. Computational and Theoretical Chemistry, 2011, 974, 143-150.	1.1	3
4652	Mechanistic insight into the DPPH radical-scavenging activity of hydroxystilbene derivatives. Computational and Theoretical Chemistry, 2011, 974, 159-162.	1.1	3
4653	Theoretical survey of the potential energy surface of Zr+acetone reaction. Computational and Theoretical Chemistry, 2011, 976, 120-129.	1.1	0
4654	Significant enhancement in efficiency of NKX-2807 Coumarin dye by applying external electric field in dye sensitizer solar cell: Theoretical study. Computational and Theoretical Chemistry, 2011, 978, 33-40.	1.1	20
4655	Monitoring corrosion and corrosion control of iron in HCl by non-ionic surfactants of the TRITON-X series – Part III. Immersion time effects and theoretical studies. Corrosion Science, 2011, 53, 1895-1909.	3.0	95
4656	The solubility of copper in high-temperature magmatic vapors: A quest for the significance of various chloride and sulfide complexes. Geochimica Et Cosmochimica Acta, 2011, 75, 2811-2827.	1.6	114
4657	Equilibrium Se isotope fractionation parameters: A first-principles study. Earth and Planetary Science Letters, 2011, 304, 113-120.	1.8	57

#	ARTICLE	IF	CITATIONS
4658	The Eltard Reaction: A DFT Study. <i>Inorganic Chemistry</i> , 2011, 50, 5833-5840.	1.9	5
4659	Tailoring the electronic structure of TiO ₂ by cation ideal, defective, and gold-promoted rutile TiO ₂ surfaces interacting with CO, H ₂ , and H ₂ O. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2795-2803.	1.1	52
4660	Theoretical Study of Medium-Sized Azacycloalkane and Dialkyl Amine Adsorption on the Fe(111) Surface. <i>Industrial & Engineering Chemistry Research</i> , 2011, 50, 7313-7318.	1.1	57
4661	Comparative study of hybrid functionals applied to structural and electronic properties of semiconductors and insulators. <i>Physical Review B</i> , 2011, 84, .	1.8	3
4662	Parallel implementation of the ab initio CRYSTAL program: electronic structure calculations for periodic systems. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2011, 467, 2112-2126.	1.1	67
4663	Intra- and Interatomic Spin Interactions by the Density Functional Theory plus U Approach: A Critical Assessment. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2795-2803.	1.0	35
4664	Origin of anomeric effect: A density functional steric analysis. <i>Journal of Chemical Physics</i> , 2011, 134, 084103.	2.3	28
4665	Can Ferric-Superoxide Act as a Potential Oxidant in P450 _{cam} ? QM/MM Investigation of Hydroxylation, Epoxidation, and Sulfoxidation. <i>Journal of the American Chemical Society</i> , 2011, 133, 5444-5452.	1.2	75
4666	Quantum-Chemical Insights into the Prediction of Charge Transport Parameters for a Naphthalenetetracarboxydiimide-Based Copolymer with Enhanced Electron Mobility. <i>Journal of the American Chemical Society</i> , 2011, 133, 19056-19059.	6.6	57
4667	Pyridazine Based Scorpionate Ligand in a Copper Boratrane Compound. <i>Inorganic Chemistry</i> , 2011, 50, 12632-12640.	6.6	95
4668	Efficient and Accurate Double-Hybrid-Meta-GGA Density Functionals Evaluation with the Extended GMTKN30 Database for General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 291-309.	1.9	43
4669	Antioxidant Potential of Glutathione: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 11269-11277.	2.3	1,035
4670	A Theoretical Study of Abiotic Methylation Reactions of Gaseous Elemental Mercury by Halogen-Containing Molecules. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5602-5608.	1.2	26
4671	Alternative Allosteric Mechanisms Can Regulate the Substrate and E2 in SUMO Conjugation. <i>Journal of Molecular Biology</i> , 2011, 406, 620-630.	1.1	13
4672	Theoretical study of the solvation of HgCl ₂ , HgClOH, Hg(OH) ₂ and HgCl ₃ ⁻ : a density functional theory cluster approach. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16772.	2.0	8
4673	Theoretical Insights into the Magnetostructural Correlations in Mn ₃ -Based Single-Molecule Magnets. <i>Inorganic Chemistry</i> , 2011, 50, 2112-2124.	1.3	32
4674	Mechanistic Studies of Wacker-Type Intramolecular Aerobic Oxidative Amination of Alkenes Catalyzed by Pd(OAc) ₂ /Pyridine. <i>Journal of Organic Chemistry</i> , 2011, 76, 1031-1044.	1.9	24
4675		1.7	78

#	ARTICLE	IF	CITATIONS
4676	Novel Pyridazine Based Scorpionate Ligands in Cobalt and Nickel Boratrane Compounds. <i>Inorganic Chemistry</i> , 2011, 50, 1991-2001.	1.9	53
4677	Calculation of the exchange coupling constants of copper binuclear systems based on spin-flip constricted variational density functional theory. <i>Journal of Chemical Physics</i> , 2011, 135, 184105.	1.2	24
4678	Synthesis and structural characterization of group 6 transition metal complexes with terminal fluoromethylidyne (CF) ligands; a DFT/NBO/NRT comparison of bonding characteristics of terminal NO, CF and CH ligands. <i>Dalton Transactions</i> , 2011, 40, 47-55.	1.6	19
4679	Spectroscopic Detection of DNA Quadruplexes by Vibrational Circular Dichroism. <i>Journal of the American Chemical Society</i> , 2011, 133, 15055-15064.	6.6	50
4680	Methemoglobinemia Caused by 8-Aminoquinoline Drugs: DFT Calculations Suggest an Analogy to H ₄ ™s Role in Nitric Oxide Synthase. <i>Journal of the American Chemical Society</i> , 2011, 133, 1172-1175.	6.6	17
4681	Synthesis and Characterization of Fe(II) η^2 -Diketonato Complexes with Relevance to Acetylacetonate Dioxygenase: Insights into the Electronic Properties of the 3-Histidine Facial Triad. <i>Inorganic Chemistry</i> , 2011, 50, 11978-11989.	1.9	28
4682	Benchmark results for empirical post-GGA functionals: Difficult exchange problems and independent tests. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19325.	1.3	83
4683	Ring-Enlargement Reactions of Donor \sim Acceptor-Substituted Cyclopropanes: Which Combinations are Most Efficient?. <i>Organic Letters</i> , 2011, 13, 1848-1851.	2.4	95
4684	Can Human Prolidase Enzyme Use Different Metals for Full Catalytic Activity?. <i>Inorganic Chemistry</i> , 2011, 50, 3394-3403.	1.9	37
4685	Computational Investigation of Amine \sim Oxygen Exciplex Formation. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10159-10165.	1.1	11
4686	2,7-Diaminofluorene-Based Organic Dyes for Dye-Sensitized Solar Cells: Effect of Auxiliary Donor on Optical and Electrochemical Properties. <i>Journal of Organic Chemistry</i> , 2011, 76, 4910-4920.	1.7	97
4687	A Diruthenium Catalyst for Selective, Intramolecular Allylic C \sim H Amination: Reaction Development and Mechanistic Insight Gained through Experiment and Theory. <i>Journal of the American Chemical Society</i> , 2011, 133, 17207-17216.	6.6	281
4688	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3567-3577.	2.3	400
4689	Water assisted dehalogenation of thionyl halides in the presence of water molecules. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 325-336.	1.1	7
4690	Validation of Relativistic DFT Approaches to the Calculation of NMR Chemical Shifts in Square-Planar Pt ²⁺ and Au ³⁺ Complexes. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3909-3923.	2.3	46
4691	An examination of density functional theories on isomerization energy calculations of organic molecules. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 851-857.	0.5	24
4692	Generalized Gradient Approximation That Recovers the Second-Order Density-Gradient Expansion with Optimized Across-the-Board Performance. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1991-1997.	2.1	171
4693	Donor-Substituted η^2 -Functionalized Porphyrin Dyes on Hierarchically Structured Mesoporous TiO ₂ Spheres. Highly Efficient Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2011, 115, 19343-19354.	1.5	130

#	ARTICLE	IF	CITATIONS
4694	Origins of the diastereoselectivity in hydrogen bonding directed Diels-Alder reactions of chiral dienes with achiral dienophiles: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 8079.	1.5	18
4695	The effect of leaving group on mechanistic preference in phosphate monoester hydrolysis. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5394.	1.5	12
4696	Theoretical studies on the inactivation mechanism of β -aminobutyric acid aminotransferase. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5162.	1.5	7
4697	Tuning of nanodiamond particles' optical properties by structural defects and surface modifications: DFT modelling. <i>Journal of Materials Chemistry</i> , 2011, 21, 18248.	6.7	26
4698	Blue-luminescent 5-(3-indolyl)oxazoles via microwave-assisted three-component coupling-cycloisomerization-Fischer indole synthesis. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 8130.	1.5	50
4699	New Design Strategy for the Two-Photon Active Material Based on Push-Pull Substituted Bisanthene Molecule. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2607-2614.	1.1	19
4700	Origins of Aryl Substituent Effects on the Stereoselectivities of Additions of Silyl Enol Ethers to a Chiral Oxazolinium Ion. <i>Organic Letters</i> , 2011, 13, 6572-6575.	2.4	8
4701	Belt-Shaped π -Systems: Relating Geometry to Electronic Structure in a Six-Porphyrin Nanoring. <i>Journal of the American Chemical Society</i> , 2011, 133, 17262-17273.	6.6	201
4702	Organocatalytic, Enantioselective Intramolecular [6 + 2] Cycloaddition Reaction for the Formation of Tricyclopentanoids and Insight on Its Mechanism from a Computational Study. <i>Journal of the American Chemical Society</i> , 2011, 133, 20175-20185.	6.6	66
4703	Addition of hydrazine to natural terpene-based isothiocyanates derivatives: density functional theory investigation. <i>Tetrahedron Letters</i> , 2011, 52, 62-64.	0.7	4
4704	Molecular structure and vibrational spectra of Benzophenone hydrazone molecule by density functional theory. <i>Computational and Theoretical Chemistry</i> , 2011, 976, 191-196.	1.1	3
4705	Gaussian and Fourier Transform (GFT) Method and Screened Hartree-Fock Exchange Potential for First-principles Band Structure Calculations. , 2011, , .		1
4706	Photosensitization Mechanisms of Triplet Excited State \hat{I}^2 -Lapachone. A Density Functional Theory Study. <i>Natural Product Communications</i> , 2011, 6, 1934578X1100601.	0.2	0
4708	Bridging quantum mechanics and structure-based drug design. <i>Frontiers in Bioscience - Landmark</i> , 2011, 16, 1619.	3.0	54
4709	Thermodynamics of ABO ₃ -Type Perovskite Surfaces. , 0, , .		4
4710	Mechanistic Study of ROS-photogeneration by Pterin. <i>Pteridines</i> , 2011, 22, 73-76.	0.5	5
4711	DFT and Cluster Model Investigation on the Adhesion of Polyethylene Terephthalate on Metals. <i>E-Journal of Surface Science and Nanotechnology</i> , 2011, 9, 251-256.	0.1	3
4712	DFT Analysis of Catalytic Urethanation. <i>Bulletin of the Chemical Society of Japan</i> , 2011, 84, 933-935.	2.0	16

#	ARTICLE	IF	CITATIONS
4713	Mechanistic Insight into the Anomalous <i>syn</i> -Selectivity Observed during the Addition of Allenylboronates to Aromatic Aldehydes. <i>Chemistry Letters</i> , 2011, 40, 1044-1046.	0.7	23
4714	A B3LYP Study on Repair of Guanyl and 8-Oxoguanyl Radical by Simultaneous Proton- and Electron-Transfer Reaction. <i>Bulletin of the Chemical Society of Japan</i> , 2011, 84, 181-190.	2.0	2
4718	Seeking for parameter-free double-hybrid functionals: The PBEO-DH model. <i>Journal of Chemical Physics</i> , 2011, 135, 024106.	1.2	226
4719	Magnetic exchange couplings evaluated with Rung 3.5 density functionals. <i>Journal of Chemical Physics</i> , 2011, 134, 214101.	1.2	14
4720	Pharmacophore Modeling and Density Functional Theory Analysis for A Series of Nitroimidazole Compounds with Antitubercular Activity. <i>Chemical Biology and Drug Design</i> , 2011, 78, 408-417.	1.5	16
4721	Europium- δ -Doped LaSi_3N_5 Ternary Nitride: Synthesis, Spectroscopy, Computed Electronic Structure and Band Gaps. <i>Journal of the American Ceramic Society</i> , 2011, 94, 4345-4351.	1.9	13
4722	Modeling of the mechanism of one-electron transfer from the perylene molecule to the oxygen molecule O_2 in the HF medium. <i>Kinetics and Catalysis</i> , 2011, 52, 192-196.	0.3	0
4723	An ab initio study of the primary hydration and proton transfer of $\text{CF}_3\text{SO}_3\text{H}$ and $\text{CF}_3\text{O}(\text{CF}_2)_2\text{SO}_3\text{H}$: Effects of the hybrid functional and inclusion of diffuse functions. <i>Solid State Ionics</i> , 2011, 199-200, 6-13.	1.3	54
4724	Synthesis and conformational analysis of new naphth[1,2-e][1,3]oxazino[3,4-c]quinazoline derivatives. <i>Tetrahedron</i> , 2011, 67, 8564-8571.	1.0	23
4725	Regio- and stereoselective cycloadditions of $(1Z,4R^-,5R^-)$ -1-arylmethylidene-4-benzoylamino-3-oxo-5-phenylpyrazolidin-1-ium-2-ides to methyl methacrylate. <i>Tetrahedron</i> , 2011, 67, 9729-9735.	1.0	13
4726	Complete investigation on the synthesis of $[\text{Ru}(\text{bpydip})\text{Cl}_2]$: the nonformation of cis isomer. <i>Tetrahedron Letters</i> , 2011, 52, 5043-5046.	0.7	2
4727	Theoretical and spectroscopic studies on the conformational equilibrium of 9-oxabispindines in solution. <i>Journal of Molecular Structure</i> , 2011, 1005, 178-185.	1.8	9
4728	Rotationally resolved electronic spectroscopy of biomolecules in the gas phase. Melatonin. <i>Journal of Molecular Spectroscopy</i> , 2011, 268, 115-122.	0.4	7
4729	A high-light-harvesting-efficiency of NKX-2593 and NKX-2883 Coumarin dyes in a local electric field: Can a local electric field enhance dye sensitizer solar cells efficiently?. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011, 225, 95-105.	2.0	13
4730	Formation, photophysical and photochemical properties of water-soluble bismuth(III) porphyrins: The role of the charge and structure. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011, 226, 23-35.	2.0	20
4731	Vibrational and electronic spectra of 9,10-dihydrobenzo(a)pyren-7(8H)-one and 7,8,9,10-tetrahydrobenzo(a)pyrene: An experimental and computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 162-171.	2.0	7
4732	Spectroscopic properties of neuroleptics: IR and Raman spectra of Risperidone (Risperdal) and of its mono- and di-protonated forms. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 631-639.	2.0	11
4733	Spectroscopic studies on the lanthanide sensitized luminescence and chemiluminescence properties of fluoroquinolone with different structure. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 375-382.	2.0	24

#	ARTICLE	IF	CITATIONS
4734	Theoretical studies on the dimerization of substituted paraphenylenediamine radical cations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 83, 368-378.	2.0	3
4735	Electron transport through molecular junctions. <i>Physics Reports</i> , 2011, 509, 1-87.	10.3	161
4736	Synthesis, characterization and DNA-binding and DNA-photocleavage studies of two Ru(II) complexes containing two main ligands and one ancillary ligand. <i>Polyhedron</i> , 2011, 30, 1953-1959.	1.0	17
4737	Influence of polarity of the medium in the saturation of the electronic properties for π -conjugated oligothiophenes. <i>Chemical Physics Letters</i> , 2011, 511, 283-287.	1.2	11
4738	Computational study on the conformations of gambogic acid. <i>Chemical Physics Letters</i> , 2011, 511, 405-412.	1.2	1
4739	Kinetic parameters of abstraction reactions of OH radical with ethylene, fluoroethylene, cis- and trans-1,2-difluoroethylene and 1,1-difluoroethylene, in the temperature range of 200-400K: Gaussian-3/B3LYP theory. <i>Chemical Physics Letters</i> , 2011, 511, 440-446.	1.2	11
4740	On the electronic structure of mono-rhenium oxide clusters: and ReO _n (n=3,4). <i>Chemical Physics Letters</i> , 2011, 512, 49-53.	1.2	15
4741	Kinetics and mechanism of the reaction of fluorine atoms with trifluoroacetic acid. <i>Chemical Physics Letters</i> , 2011, 512, 172-177.	1.2	9
4742	Theoretical and experimental investigation of the C ₂ H+SO ₂ reaction over the range T=295-800K. <i>Chemical Physics Letters</i> , 2011, 513, 201-207.	1.2	5
4743	Photoinduced intramolecular charge transfer process of betaine pyridinium: A theoretical spectroscopic study. <i>Chemical Physics Letters</i> , 2011, 515, 42-48.	1.2	13
4744	Frozen density embedding calculations with the orbital-dependent localized Hartree-Fock Kohn-Sham potential. <i>Chemical Physics Letters</i> , 2011, 518, 114-118.	1.2	20
4745	Poly(oxyethylene) electrolytes based on lithium nitrophenyl sulfonamide and hexanitrodiphenylamide. <i>Electrochimica Acta</i> , 2011, 57, 20-26.	2.6	6
4746	Nanoscale structure and morphology of thin films of poly(2-chloroxylylene) synthesized by the CVD method on different liquids. <i>European Polymer Journal</i> , 2011, 47, 1725-1735.	2.6	3
4747	Computational study on the mechanisms of action of the potential anticancer drug trans-isopropylaminedimethylaminedichloroplatinum (trans-IPADMADP) and its cis isomer with DNA purine bases. <i>Inorganica Chimica Acta</i> , 2011, 376, 44-56.	1.2	9
4748	Re(V) complexes formed by metal-assisted solvolysis of di-(2-pyridyl)ketone: Synthesis, X-ray studies, redox behavior and DFT calculations. <i>Inorganica Chimica Acta</i> , 2011, 376, 105-111.	1.2	10
4749	Novel sandwich-type dimetallocenes: Toward promising candidate media for high-capacity hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2011, 36, 11810-11814.	3.8	15
4750	Electron transfer pathways in cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2011, 1807, 1305-1313.	0.5	34
4751	Effect of different C3-aryl substituents on the antioxidant activity of 4-hydroxycoumarin derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 6233-6238.	1.4	39

#	ARTICLE	IF	CITATIONS
4752	Photophysical and photochemical properties of the pharmaceutical compound salbutamol in aqueous solutions. <i>Chemosphere</i> , 2011, 83, 1513-1523.	4.2	25
4753	Time-dependent density functional theory applied to ligand-field excitations and their circular dichroism in some transition metal complexes. <i>Chemical Physics</i> , 2011, 391, 92-100.	0.9	21
4754	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6670.	1.3	1,627
4755	Modeling Molecular Acidity with Electronic Properties and Hammett Constants for Substituted Benzoic Acids. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14697-14707.	1.1	35
4756	Optical Rotation Calculated with Time-Dependent Density Functional Theory: The OR45 Benchmark. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10930-10949.	1.1	110
4757	Revisiting the Atomic Natural Orbital Approach for Basis Sets: Robust Systematic Basis Sets for Explicitly Correlated and Conventional Correlated <i>ab initio</i> Methods?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 33-43.	2.3	274
4758	Electronic Structure of Pure and N-Doped TiO ₂ Nanocrystals by Electrochemical Experiments and First Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 6381-6391.	1.5	118
4759	Influence of Triplet Instabilities in TDDFT. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3578-3585.	2.3	285
4760	Mechanism of the Palladium-Catalyzed Addition of Arylboronic Acids to Enones: A Computational Study. <i>Journal of Organic Chemistry</i> , 2011, 76, 4905-4909.	1.7	46
4761	Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional. <i>Physical Review B</i> , 2011, 84, .	1.1	281
4762	Synthesis of Pyrazoles via Electrophilic Cyclization. <i>Journal of Organic Chemistry</i> , 2011, 76, 6726-6742.	1.7	125
4763	Pyridazine- versus Pyridine-Based Tridentate Ligands in First-Row Transition Metal Complexes. <i>Inorganic Chemistry</i> , 2011, 50, 7478-7488.	1.9	27
4764	Electronic structure and absorption spectra of supramolecular complexes of a fullerene crown ether with a π -extended TTF derivative. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11965.	1.3	17
4765	Method to include explicit correlations into density-functional calculations based on density-matrix functional theory. <i>Physical Review B</i> , 2011, 84, .	1.1	16
4766	Electronic Effects of <i>para</i> -Substitution on the Melting Points of TAILs. <i>Chemistry - an Asian Journal</i> , 2011, 6, 863-867.	1.7	35
4767	Assessing computationally efficient isomerization dynamics: \hat{T} SCF density-functional theory study of azobenzene molecular switching. <i>Journal of Chemical Physics</i> , 2011, 135, 224303.	1.2	53
4768	The Contribution of Theoretical Chemistry to the Drug Design in Photodynamic Therapy. , 2011, , 121-134.		0
4769	Key Building Block of Photoresponsive Biomimetic Systems. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1232-1242.	1.2	6

#	ARTICLE	IF	CITATIONS
4770	The Nature of the Interaction of Organoselenium Molecules with Diiodine. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10069-10077.	1.1	19
4771	Time-Dependent Density Functional Theory Investigation of the Electronic Spectra of Hexanuclear Chalcogenide Rhenium(III) Clusters. <i>Journal of Physical Chemistry A</i> , 2011, 115, 211-218.	1.1	12
4772	Predicting Michael-acceptor reactivity and toxicity through quantum chemical transition-state calculations. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 8400.	1.5	69
4773	Optical excitations in stoichiometric uncapped ZnS nanostructures. <i>Nanoscale</i> , 2011, 3, 3780.	2.8	20
4774	Investigation of the photoinduced electron injection processes for p-type triphenylamine-sensitized solar cells. <i>Energy and Environmental Science</i> , 2011, 4, 4537.	15.6	63
4775	Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. <i>Frontiers of Chemistry in China: Selected Publications From Chinese Universities</i> , 2011, 6, 269-279.	0.4	22
4776	Experimental and theoretical study on 6-substituted pyridoxine derivatives. Synthesis of cyclic 2,4,5,6-tetrakis-(hydroxymethyl)pyridin-3-ol acetonides. <i>Russian Journal of Organic Chemistry</i> , 2011, 47, 100-108.	0.3	6
4777	Calculation of geometric parameters of macrocyclic metal chelates formed by template synthesis in tertiary systems M(II) ion-ethanedithioamide-formaldehyde-ammonia. <i>Russian Journal of Inorganic Chemistry</i> , 2011, 56, 223-231.	0.3	26
4778	Calculation of geometric parameters and energies of macrocyclic metal chelates in the ternary M(II) ion-thiocarbamoylmethanamide-formaldehyde systems. <i>Russian Journal of Inorganic Chemistry</i> , 2011, 56, 1935-1942.	0.3	27
4779	The relative stability of macrotricyclic metal complexes in M(II)-thiocarbohydrazide-acetone (M = Mn, Ni, Cu, Zn). <i>Journal of Physical Chemistry A</i> , 2011, 85, 152-155.	0.1	10
4780	Stability of isomeric chelates in M(II)-thiocarbamoylmethanamide-ethandial systems according to the DFT B3LYP method (M = Mn, Fe, Co, Ni, Cu, Zn). <i>Russian Journal of Physical Chemistry A</i> , 2011, 85, 1475-1477.	0.1	7
4781	Prediction of Charge Mobility in Amorphous Organic Materials through the Application of Hopping Theory. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2556-2567.	2.3	24
4782	How Well Can Modern Density Functionals Predict Internuclear Distances at Transition States?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1667-1676.	2.3	156
4783	Exchange functional by a range-separated exchange hole. <i>Physical Review A</i> , 2011, 83, .	1.0	5
4784	A molecular dynamics investigation of structure and dynamics of SDS and SDBS micelles. <i>Soft Matter</i> , 2011, 7, 9148.	1.2	99
4785	Density Functional Theory Modeling of PbSe Nanoclusters: Effect of Surface Passivation on Shape and Composition. <i>Journal of Physical Chemistry C</i> , 2011, 115, 11382-11389.	1.5	37
4786	Density Functional Theory for Reaction Energies: Test of Meta and Hybrid Meta Functionals, Range-Separated Functionals, and Other High-Performance Functionals. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 669-676.	2.3	190
4787	Density Functional Calculations. , 2011, , 445-519.		3

#	ARTICLE	IF	CITATIONS
4788	Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16987.	1.3	301
4789	Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2810-2817.	2.1	864
4790	DNA insertion in and wrapping around carbon nanotubes. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 902-919.	6.2	6
4791	Rational design, synthesis and biological evaluations of amino-noscapine: a high affinity tubulin-binding noscapinoid. <i>Journal of Computer-Aided Molecular Design</i> , 2011, 25, 443-454.	1.3	53
4792	A QM/MM study of the binding of RAPTA ligands to cathepsin B. <i>Journal of Computer-Aided Molecular Design</i> , 2011, 25, 729-742.	1.3	36
4793	Calculation of chemical shift anisotropy in proteins. <i>Journal of Biomolecular NMR</i> , 2011, 51, 303-312.	1.6	41
4794	Electronic Properties and Chemical Bonding of O-Rich Clusters $M\text{O}_7^-$ (M, $\text{M}=\text{V}, \text{Nb}, \text{Ta}$). <i>Journal of Cluster Science</i> , 2011, 22, 397-404.	1.7	1
4795	Polymorphism and Intramolecular Proton Transfer in Fluoroquinolone Compounds. <i>Journal of Fluorescence</i> , 2011, 21, 2117-2122.	1.3	6
4796	Finding minimum energy reaction paths on ab initio potential energy surfaces using the fast marching method. <i>Journal of Mathematical Chemistry</i> , 2011, 49, 1291-1301.	0.7	3
4797	Newton trajectories for finding stationary points on molecular potential energy surfaces. <i>Journal of Mathematical Chemistry</i> , 2011, 49, 1915-1927.	0.7	12
4798	Electronic properties of poly(thiophene-3-methyl acetate). <i>Journal of Polymer Research</i> , 2011, 18, 1509-1517.	1.2	17
4799	Theoretical study on the atmospheric formation of sulfur trioxide as the primary agent for acid rain. <i>Structural Chemistry</i> , 2011, 22, 817-822.	1.0	10
4800	A theoretical study on the mechanism of a novel one-carbon unit transfer reaction. <i>Structural Chemistry</i> , 2011, 22, 901-907.	1.0	1
4801	Half-sandwich scorpionate nickel complexes with aliphatic dicarboxylic acid co-ligands. <i>Transition Metal Chemistry</i> , 2011, 36, 621-629.	0.7	3
4802	Metalloporphyrin intercalation in liposome membranes: ESR study. <i>Journal of Biological Inorganic Chemistry</i> , 2011, 16, 173-181.	1.1	34
4803	Oxygen cleavage with manganese and iron in ribonucleotide reductase from <i>Chlamydia trachomatis</i> . <i>Journal of Biological Inorganic Chemistry</i> , 2011, 16, 553-565.	1.1	26
4804	Hydroxyl group as a substituent with varying electronic properties: Effect of strength of H-bonding on charge density changes in $\text{Ph}^{\oplus}\text{OH}^{\ominus}\text{F}^{\oplus}$ complexes. <i>Journal of Molecular Modeling</i> , 2011, 17, 125-131.	0.8	4
4805	Hybridization-displaced charges for amino-acids: a new model using two point charges per atom along with bond-center charges. <i>Journal of Molecular Modeling</i> , 2011, 17, 1435-1444.	0.8	8

#	ARTICLE	IF	CITATIONS
4806	Supramolecular synthon pattern in solid cloiquinol and cloiquine (APIs of antibacterial, antifungal,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Journal of Molecular Modeling, 2011, 17, 1781-1800.	0.8	15
4807	Light activation of the isomerization and deprotonation of the protonated Schiff base retinal. Journal of Molecular Modeling, 2011, 17, 2539-2547.	0.8	15
4808	Role of physicochemical properties in the activation of peroxisome proliferator-activated receptor Î. Journal of Molecular Modeling, 2011, 17, 2549-2558.	0.8	12
4809	Effect of metal ions (Ni ²⁺ , Cu ²⁺ and Zn ²⁺) and water coordination on the structure of L-phenylalanine, L-tyrosine, L-tryptophan and their zwitterionic forms. Journal of Molecular Modeling, 2011, 17, 3117-3128.	0.8	62
4810	Synthesis, characterization, and optical properties of 2-amino-4-aryl-6-(9,9- ϵ^2 -spirobifluoren-2-yl)pyrimidines. Monatshefte FÃ¼r Chemie, 2011, 142, 907-916.	0.9	6
4811	Investigation on specific adsorption of hydrogen on lithium-doped mesoporous silica. Adsorption, 2011, 17, 211-218.	1.4	9
4812	Dual-level direct dynamics studies on the hydrogen abstraction reactions of fluorine atoms with CF ₃ CH ₂ X(X=F, Cl). Theoretical Chemistry Accounts, 2011, 128, 183-189.	0.5	13
4813	The reaction between HO and (H ₂ O) _n (n=1, 3) clusters: reaction mechanisms and tunneling effects. Theoretical Chemistry Accounts, 2011, 128, 579-592.	0.5	37
4814	On the mechanism of the N-glycosidic bond hydrolysis of 2- ϵ^2 -deoxyguanosine: insights from first principles calculations. Theoretical Chemistry Accounts, 2011, 128, 619-626.	0.5	14
4815	Charge transport and electronic properties of N-heteroquinones: quadruple weak hydrogen bonds and strong Î€-Î€ stacking interactions. Theoretical Chemistry Accounts, 2011, 128, 257-264.	0.5	20
4816	Theoretical study of one- and two-photon absorption properties of pyrene derivatives. Theoretical Chemistry Accounts, 2011, 128, 265-274.	0.5	9
4817	Bonding in cationic MOH _n + (M=Al, Hf, Rn; n=0, 2): DFT performances and periodic trends. Theoretical Chemistry Accounts, 2011, 129, 389-399.	0.5	40
4818	Assessment of higher-order spin-orbit effects on electronic g-tensors of d 1 transition-metal complexes by relativistic two- and four-component methods. Theoretical Chemistry Accounts, 2011, 129, 715-725.	0.5	39
4819	A theoretical study on magnesium ion-selective two-photon fluorescent probe based on benzo [h] chromene derivatives. Theoretical Chemistry Accounts, 2011, 130, 61-68.	0.5	10
4820	Assessment of theoretical procedures for hydrogen-atom abstraction by chlorine, and related reactions. Theoretical Chemistry Accounts, 2011, 130, 251-260.	0.5	37
4821	Computational study on the partial dechlorination of the pesticide chloropicrin by sulfur species. Theoretical Chemistry Accounts, 2011, 130, 955-963.	0.5	3
4822	Photoionization cross-section weighted DFT simulations as promising tool for the investigation of the electronic structure of open shell metal-phthalocyanines. Analytical and Bioanalytical Chemistry, 2011, 400, 673-678.	1.9	17
4823	Intra-cluster proton transfer in anilide(HF) _n (n=1-4): Can the size of HF cluster influence the N-H...F...H switching. Journal of Fluorine Chemistry, 2011, 132, 459-467.	0.9	9

#	ARTICLE	IF	CITATIONS
4824	Theoretical study of new acceptor and donor molecules based on polycyclic aromatic hydrocarbons. <i>Journal of Molecular Spectroscopy</i> , 2011, 265, 95-101.	0.4	27
4825	Host-guest complex of cypermethrin with β -cyclodextrin: A spectroscopy and theoretical investigation. <i>Journal of Molecular Structure</i> , 2011, 990, 244-252.	1.8	28
4826	From the X-rays to a reliable low cost computational structure of caffeic acid: DFT, MP2, HF and integrated molecular dynamics-X-ray diffraction approach to condensed phases. <i>Journal of Molecular Structure</i> , 2011, 994, 87-96.	1.8	11
4827	Prediction of protein ^{13}C NMR chemical shifts using a combination scheme of statistical modeling and quantum-mechanical analysis. <i>Journal of Molecular Structure</i> , 2011, 995, 163-172.	1.8	10
4828	Applications and validations of the Minnesota density functionals. <i>Chemical Physics Letters</i> , 2011, 502, 1-13.	1.2	662
4829	A conceptually improved TD-DFT approach for predicting the maximum absorption wavelength of cyanine dyes. <i>Dyes and Pigments</i> , 2011, 90, 114-118.	2.0	30
4830	Coumarin dyes containing low-band-gap chromophores for dye-sensitised solar cells. <i>Dyes and Pigments</i> , 2011, 90, 304-310.	2.0	126
4831	Quantum chemical calculation on the potential energy surface of H_2CO_3 and its implication for martian chemistry. <i>Icarus</i> , 2011, 214, 228-235.	1.1	10
4832	Experimental and theoretical study of a Diels-Alder reaction between a sugar-derived nitroalkene and cyclopentadiene. <i>Carbohydrate Research</i> , 2011, 346, 460-464.	1.1	8
4833	Crystallization from solutions containing multiple conformers: A new modeling approach for solubility and supersaturation. <i>Chemical Engineering Science</i> , 2011, 66, 88-102.	1.9	34
4834	Theoretical study of the excitation spectrum of azomethane. <i>Chemical Physics</i> , 2011, 380, 9-16.	0.9	13
4835	Transition Metal Ions: Charge Carriers that Mediate the Electron Capture Dissociation Pathways of Peptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2011, 22, 2232-2245.	1.2	25
4836	Electron-Capture and -Transfer Dissociation of Peptides Tagged with Tunable Fixed-Charge Groups: Structures and Dissociation Energetics. <i>Journal of the American Society for Mass Spectrometry</i> , 2011, 22, 13-30.	1.2	11
4837	Formation of Peptide Radical Cations ($\text{M}+\dot{\text{A}}$) in Electron Capture Dissociation of Peptides Adducted with Group IIB Metal Ions. <i>Journal of the American Society for Mass Spectrometry</i> , 2011, 22, 233-244.	1.2	22
4838	Dipole-Guided Electron Capture Causes Abnormal Dissociations of Phosphorylated Pentapeptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2011, 22, 731-751.	1.2	36
4839	Development, evaluation and application of 3D QSAR Pharmacophore model in the discovery of potential human renin inhibitors. <i>BMC Bioinformatics</i> , 2011, 12, S4.	1.2	52
4840	The curing retardation and mechanism of high temperature vulcanizing silicone rubber filled with superconductive carbon blacks. <i>Polymer Engineering and Science</i> , 2011, 51, 170-178.	1.5	9
4841	Calculation of semiconductor band structures and defects by the screened exchange density functional. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 537-546.	0.7	26

#	ARTICLE	IF	CITATIONS
4842	Defect levels through hybrid density functionals: Insights and applications. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 775-789.	0.7	253
4843	Predicting polaronic defect states by means of generalized Koopmans density functional calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1052-1060.	0.7	59
4844	Advances in electronic structure methods for defects and impurities in solids. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 19-27.	0.7	66
4845	Accurate treatment of solids with the HSE screened hybrid. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 767-774.	0.7	258
4846	Which electronic structure method for the study of defects: A commentary. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1547-1558.	0.7	39
4847	A computational study of CiX ($X = H, C, F, Cl$) bond dissociation enthalpies (BDEs) in polyhalogenated methanes and ethanes. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 65-73.	0.9	18
4848	CiH bond activation of ethylene by bare neutral palladium and platinum atoms: a theoretical investigation. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 292-298.	0.9	6
4849	The photoinduced reaction of 2-iodothiophene in solutions of n -heptane, dichloromethane and methanol. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 398-406.	0.9	5
4850	Fundamental properties of N -alkenylaziridines" implications for the design of new reactions and organocatalysts. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 445-449.	0.9	1
4851	Computational (solute+solvent cluster+PCM) study of medium effects on the experimental ^{13}C and 1H NMR chemical shifts of lactones and lactams. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 1209-1221.	0.9	3
4852	Reactivity of carbene-phosphine dimers: proton affinity revisited. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 929-936.	0.9	16
4853	Dependence of collision-induced dissociation energy on molecular degrees of freedom as a means to assess relative binding affinity in multivalent complexes. <i>Rapid Communications in Mass Spectrometry</i> , 2011, 25, 2299-2306.	0.7	3
4854	Proton Conductivity of SO_3 -Functionalized Benzene-Periodic Mesoporous Organosilica. <i>Small</i> , 2011, 7, 1086-1097.	5.2	36
4855	A theoretical analysis of topography and molecular parameters of the $CFCl_3 \cdots O_3$ complex: Linear and bifurcate halogen-oxygen bonding interactions. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 111-116.	1.0	22
4856	Structure and optical spectra of bis(pyrrolidyl)methyleneamine complexes: A DFT and TDDFT study of the self-assembly complexes of bis(pyrrolidyl)methyleneamine ligands linked by alkyl spacers with Cu(II). <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2099-2108.	1.0	1
4857	A DFT study of determination of the reactive sites of the acetylcholine and its agonists: In the gas phase and dielectric medium. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2464-2475.	1.0	23
4858	Gas-phase reaction mechanism of Pd^+ with CH_3CHO : A density functional theoretical study. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2359-2365.	1.0	0
4859	A mechanism of the 1,3-dipolar cycloaddition between the hydrogen nitril HNO_2 and acetylene HCCH: The electron localization function study on evolution of the chemical bonds. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2378-2389.	1.0	9

#	ARTICLE	IF	CITATIONS
4860	Theoretical investigation on chiral cinchona alkaloid salts-catalyzed asymmetric epoxidation of cyclic enones. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2874-2881.	1.0	6
4861	The gas-phase H-abstraction reactions of CCl_3H with CX_2 ($\text{X}_1\text{X}_2 = \text{HF}, \text{HCl}, \text{HBr}, \text{HI}, \text{FF}, \text{ClCl}, \text{BrBr}, \text{and I I}$), a DFT study. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3048-3056.	1.0	6
4862	New nonsteroidal anti-inflammatory molecules with reduced photodegradation side effects and enhanced COX-2 selectivity. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1184-1195.	1.0	6
4863	Advances in local hybrid exchange-correlation functionals: from thermochemistry to magnetic-resonance parameters and hyperpolarizabilities. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2625-2638.	1.0	42
4864	Modeling of plastic scintillation composition of poly(methyl methacrylate)-naphthalene-POPOP. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2540-2544.	1.0	0
4865	DFT and <i>Ab initio</i> computational study on the reactivity sites of the GABA and its agonists, such as CACA, TACA, DABA, and muscimol: In the gas phase and dielectric media. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3938-3948.	1.0	23
4866	Study of geometries and electronic properties of AgSi_n clusters using DFT/TB. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1680-1693.	1.0	16
4867	The reaction mechanism of the gas-phase thermal decomposition kinetics of neopentyl halides: A DFT study. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 4011-4019.	1.0	3
4868	Kinetics of the hydrogen abstraction $\text{R}^\bullet\text{OH} + \text{H} \rightarrow \text{R}^\bullet\text{OH} + \text{H}_2$ reaction class: An application of the reaction class transition state theory. <i>International Journal of Chemical Kinetics</i> , 2011, 43, 78-98.	1.0	19
4869	Theoretical study of the mechanism for the gas-phase pyrolysis kinetics of 2-methylbenzyl chloride. <i>International Journal of Chemical Kinetics</i> , 2011, 43, 537-546.	1.0	4
4870	Structure and dissociation characteristics of metal chloride anion clusters containing redox-active metal ions studied by laser desorption and electrospray ionization mass spectrometry and <i>ab initio</i> calculations. <i>Journal of Mass Spectrometry</i> , 2011, 46, 223-229.	0.7	9
4871	JMS Letters. <i>Journal of Mass Spectrometry</i> , 2011, 46, 1199-1202.	0.7	1
4872	Protonation sites and dissociation mechanisms of <i>t</i> -butylcarbamates in tandem mass spectrometric assays for newborn screening. <i>Journal of Mass Spectrometry</i> , 2011, 46, 1089-1098.	0.7	15
4873	DFT calculations of ^{31}P spin-spin coupling constants and chemical shift in dioxaphosphorinanes. <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 399-404.	1.1	19
4874	Isotopic effect on tautomeric behavior of 5-(2,6-disubstituted-aryloxy)-tetrazoles. <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 592-599.	1.1	6
4875	DFT studies of ESR parameters for Ni O centered radicals, <i>N</i> -alkoxyaminy and aminoxyl radicals. <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 603-610.	1.1	7
4876	Spectroscopic and Photophysical Studies of Charge-Transfer in a Cd_8 Thiolate Cluster Complex Containing a Coordinated <i>N</i> -Methyl-4,4'-bipyridinium Ligand. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 660-665.	1.0	14
4877	Homopolynuclear TII and Heteropolynuclear AuI-TII Complexes with Organodisilone Ligands: Activation of Luminescence by Intermetallic Interactions. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 2288-2297.	1.0	20

#	ARTICLE	IF	CITATIONS
4878	The Effect of Strain on the Rh ^I -Catalyzed Rearrangement of Allylamines. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 553-561.	1.2	3
4879	(+)-Flavipucine, the Missing Member of the Pyridione Epoxide Family of Fungal Antibiotics. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 5156-5162.	1.2	31
4880	Synthesis, Electrochemical and Optical Absorption Properties of New Perylene ^{3,4:9,10} -bis(dicarboximide) and Perylene ^{3,4:9,10} -bis(benzimidazole) Derivatives. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 5427-5440.	1.2	63
4881	Bis-Donor-Bis-Acceptor Tribranched Organic Sensitizers for Dye-Sensitized Solar Cells. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 6195-6205.	1.2	50
4882	1,3-Benzyl Migration in Iminium Ions: Evidence for a Fast Free-Radical Chain Reaction. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 7355-7365.	1.2	9
4883	Rotationally Resolved Electronic Spectroscopy of 1,4-Benzodioxan: The Anomeric Effect in the Ground and Electronically Excited State. <i>ChemPhysChem</i> , 2011, 12, 2035-2041.	1.0	2
4884	Acetylene...Furan Trimer Formation at 0.37 K as a Model for Ultracold Aggregation of Non- and Weakly Polar Molecules. <i>ChemPhysChem</i> , 2011, 12, 2009-2017.	1.0	7
4885	On the Photophysics of 1,6-Diphenyl-1,3,5-Hexatriene Isomers and Rotamers. <i>ChemPhysChem</i> , 2011, 12, 1872-1879.	1.0	10
4886	Reduction Potentials and Acidity Constants of Mn Superoxide Dismutase Calculated by QM/MM Free-Energy Methods. <i>ChemPhysChem</i> , 2011, 12, 3337-3347.	1.0	38
4887	Theoretical Study of the Photochemistry of a Reversible Three-State Bis-Thioxanthylidene Molecular Switch. <i>ChemPhysChem</i> , 2011, 12, 3348-3353.	1.0	9
4888	Ultrafast Dynamics of UV-Excited Imidazole. <i>ChemPhysChem</i> , 2011, 12, 3365-3375.	1.0	33
4889	The first branching point in porphyrin biosynthesis: A systematic docking, molecular dynamics and quantum mechanical/molecular mechanical study of substrate binding and mechanism of uroporphyrinogen ^{III} decarboxylase. <i>Journal of Computational Chemistry</i> , 2011, 32, 822-834.	1.5	17
4890	Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. <i>Journal of Computational Chemistry</i> , 2011, 32, 1824-1838.	1.5	26
4891	Assessment of TD-DFT and TD-CF based approaches for the prediction of exciton coupling parameters, potential energy curves, and electronic characters of electronically excited aggregates. <i>Journal of Computational Chemistry</i> , 2011, 32, 1971-1981.	1.5	70
4892	A computational study of unique properties of pillar[5]quinones: Self-assembly to tubular structures and potential applications as electron acceptors and anion recognizers. <i>Journal of Computational Chemistry</i> , 2011, 32, 2716-2726.	1.5	30
4893	Different properties for poly(3,4-ethylenedioxythiophene) films derived from single or multiple polymerization steps. <i>Journal of Applied Polymer Science</i> , 2011, 121, 1982-1991.	1.3	17
4894	A theoretical investigation on the properties of the new poly(vinylcarbazole)- <i>b</i> -methylthiophene (PVK- <i>b</i> -MeT) synthesized graft copolymer. <i>Journal of Applied Polymer Science</i> , 2011, 122, 2391-2402.	1.3	13
4897	Reversible Binding of Ethylene to Silylene-Phosphine Complexes at Room Temperature. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 10414-10416.	7.2	94

#	ARTICLE	IF	CITATIONS
4898	Dispersion and Back-Donation Gives Tetracoordinate [Pd(PPh ₃) ₄]. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11794-11797.	7.2	77
4899	Enhanced Functionality for Donor-Acceptor Oligothiophenes by means of Inclusion of BODIPY: Synthesis, Electrochemistry, Photophysics, and Model Chemistry. <i>Chemistry - A European Journal</i> , 2011, 17, 498-507.	1.7	63
4900	Metal-Free Dehydration of Glucose to 5-(Hydroxymethyl)furfural in Ionic Liquids with Boric Acid as a Promoter. <i>Chemistry - A European Journal</i> , 2011, 17, 1456-1464.	1.7	177
4901	Dinuclear Copper(I) Thiolate Complexes with a Bridging Noninnocent PNP Ligand. <i>Chemistry - A European Journal</i> , 2011, 17, 3850-3854.	1.7	59
4902	Chloropupukeanolides: Cytotoxic Pupukeanane Chlorides with a Spiroketal Skeleton from <i>Pestalotiopsis fici</i> . <i>Chemistry - A European Journal</i> , 2011, 17, 2604-2613.	1.7	78
4903	Investigation of Aromaticity and Photophysical Properties in [18]/[20] Porphycene Derivatives. <i>Chemistry - A European Journal</i> , 2011, 17, 7882-7889.	1.7	23
4904	Rhodium-Catalyzed Highly Enantioselective Addition of Arylboronic Acids to 2-Nitrostyrenes by <i>tert</i> -Butanesulfinylphosphine Ligand. <i>Chemistry - A European Journal</i> , 2011, 17, 5242-5245.	1.7	70
4905	Chemical Modulation of Peptoids: Synthesis and Conformational Studies on Partially Constrained Derivatives. <i>Chemistry - A European Journal</i> , 2011, 17, 7927-7939.	1.7	33
4906	Chiral Monofluorobenzyl Carbanions: Synthesis of Enantiopure ¹⁸ F-Fluorinated ¹⁸ F-Phenylethylamines. <i>Chemistry - A European Journal</i> , 2011, 17, 6142-6147.	1.7	23
4907	Synthesis, Electronic, and Electro-Optical Properties of Emissive Solvatochromic Phenothiazinyl Merocyanine Dyes. <i>Chemistry - A European Journal</i> , 2011, 17, 9984-9998.	1.7	67
4908	Efficient Epoxidation of Electron-Deficient Alkenes with Hydrogen Peroxide Catalyzed by [P ₁₀ O ₃₈ V ₂ (H ₂ O) ₂] ³⁻ . <i>Chemistry - A European Journal</i> , 2011, 17, 7549-7559.	1.7	73
4909	Selectivity in the Addition Reactions of Organometallic Reagents to Aziridine-2-carboxaldehydes: The Effects of Protecting Groups and Substitution Patterns. <i>Chemistry - A European Journal</i> , 2011, 17, 12326-12339.	1.7	16
4910	New Perspectives on Iron-Ligand Vibrations of Oxyheme Complexes. <i>Chemistry - A European Journal</i> , 2011, 17, 11178-11185.	1.7	21
4911	Gas-Phase Radical Radical Reaction Dynamics of O(³ P)+C ₂ H ₃ +C ₂ H ₂ +OH. <i>Chemistry - A European Journal</i> , 2011, 17, 11410-11414.	1.7	2
4912	Enantioselective and Diastereoselective Tsuji-Trost Allylic Alkylation of Lactones: An Experimental and Computational Study. <i>Chemistry - A European Journal</i> , 2011, 17, 11243-11249.	1.7	32
4913	Does a Concerted Non-Insertive Mechanism Prevail over a σ -Insertive Mechanism in Catalytic Cyclohydroamination by Magnesium Tris(oxazolonyl)phenylborate Compounds? A Computational Study. <i>Chemistry - A European Journal</i> , 2011, 17, 14974-14986.	1.7	34
4914	Blue Emitting Spiro Terfluorene-Indenofluorene Isomers: A Structure-Properties Relationship Study. <i>Chemistry - A European Journal</i> , 2011, 17, 14031-14046.	1.7	51
4915	Palladium-Catalyzed Allylic Sulfinylation and the Mislow-Braverman-Evans Rearrangement. <i>Chemistry - A European Journal</i> , 2011, 17, 13963-13965.	1.7	5

#	ARTICLE	IF	CITATIONS
4916	Theoretical investigation on properties of the ground and lowest excited states of a red emitter with donor- π -acceptor structure. <i>Chemical Physics</i> , 2011, 381, 100-104.	0.9	14
4917	Effect of Fe-Pd bimetallic nanoparticles on <i>Sphingomonas</i> sp. PH-07 and a nano-bio hybrid process for triclosan degradation. <i>Bioresource Technology</i> , 2011, 102, 6019-6025.	4.8	58
4918	Towards more specific O6-methylguanine-DNA methyltransferase (MGMT) inactivators. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 1658-1665.	1.4	6
4919	DFT/TD-DFT investigation of optical absorption spectra, electron affinities, and ionization potentials of mono-nitrated benzanthrones. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 40-50.	1.1	19
4920	The reaction: Current status and prospective work. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 291-297.	1.1	15
4921	Theoretical approach of the mechanism of the reactions of chlorine atoms with aliphatic aldehydes. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 321-327.	1.1	9
4922	Gas phase reactions of nitromethyl carbanion with CHCl ₃ and CCl ₄ : A theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2011, 964, 304-309.	1.1	5
4923	Reaction of acetaldehyde with zirconium: A density functional theoretical study. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 60-67.	1.1	4
4924	Density functional study for the C-F bond activation of the reaction of [Pt(PCy ₃) ₂] with C ₆ F ₆ . <i>Computational and Theoretical Chemistry</i> , 2011, 965, 92-100.	1.1	12
4925	On the mechanism of AuCl ₃ -catalyzed synthesis of highly substituted furans from 2-(1-alkynyl)-2-alken-1-ones with nucleophiles: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 180-185.	1.1	10
4926	Quantum mechanical modeling of a tripodal [2]rotaxane and its binding to TiO ₂ . <i>Computational and Theoretical Chemistry</i> , 2011, 966, 180-185.	1.1	4
4927	Theoretical mechanisms of the superoxide radical anion catalyzed by the nickel superoxide dismutase. <i>Computational and Theoretical Chemistry</i> , 2011, 966, 357-363.	1.1	10
4928	Accurate finite element method for atomic calculations based on density functional theory and Hartree-Fock method. <i>Computer Physics Communications</i> , 2011, 182, 1245-1252.	3.0	11
4929	AIM and BET approach for ionic and covalent bond evolution in reaction of hydrogen elimination from ammonia and lithium hydride. <i>Chemical Physics Letters</i> , 2011, 501, 587-593.	1.2	8
4930	Experimental and PCM/TD-DFT investigation on the absorption and emission spectra of a light emitting material in various solvents. <i>Chemical Physics Letters</i> , 2011, 503, 75-79.	1.2	17
4931	Broken-symmetry natural orbital (BSNO)-Mk-MRCC study on the exchange coupling in the binuclear copper(II) compounds. <i>Chemical Physics Letters</i> , 2011, 505, 11-15.	1.2	20
4932	The unique bonding characteristics of beryllium and the Group IIA metals. <i>Chemical Physics Letters</i> , 2011, 506, 1-14.	1.2	68
4933	Oxygen bound iodine (O-I): The Electron Localization Function (ELF) study on bonding in cis- and trans-IONO. <i>Chemical Physics Letters</i> , 2011, 506, 15-21.	1.2	6

#	ARTICLE	IF	CITATIONS
4934	Electronic ground state conformers of β -carotene and their role in ultrafast spectroscopy. <i>Chemical Physics Letters</i> , 2011, 506, 122-127.	1.2	40
4935	Stability and proton transfer in DNA base pairs of AMD473â€“DNA adduct. <i>Chemical Physics Letters</i> , 2011, 508, 295-299.	1.2	10
4936	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. <i>Chemical Physics Letters</i> , 2011, 510, 165-178.	1.2	353
4937	Co(II) complexes with tripodal N-donor ligands: Thermodynamics of formation in anaerobic conditions and oxygen binding. <i>Inorganica Chimica Acta</i> , 2011, 367, 120-126.	1.2	11
4938	Proper and improper aminoketyl radicals in electron-based peptide dissociations. <i>International Journal of Mass Spectrometry</i> , 2011, 301, 55-61.	0.7	30
4939	Dissociative electron attachment to carbonyl fluoride, F ₂ CO. <i>International Journal of Mass Spectrometry</i> , 2011, 303, 125-128.	0.7	5
4940	Rotationally resolved electronic spectroscopy of 2,3-bridged indole derivatives: Tetrahydrocarbazole. <i>Journal of Molecular Structure</i> , 2011, 993, 2-8.	1.8	7
4941	Synthesis, DNA-binding, DNA-photocleavage and antioxidant activity of ruthenium(II) complex containing triazine ring ligand: [Ru(dmb) ₂ (pdta)](ClO ₄) ₂ . <i>Journal of Molecular Structure</i> , 2011, 990, 197-203.	1.8	25
4942	Are the structures of (5n8) clusters featured by two connected carbons or by two separated carbons?. <i>Journal of Molecular Structure</i> , 2011, 1000, 4-9.	1.8	0
4943	Experimental and theoretical study of vibrational spectra of 3-nitrofluoranthene. <i>Journal of Molecular Structure</i> , 2011, 999, 22-28.	1.8	7
4944	Trichloroisocyanuric acid in 98% sulfuric acid: A superelectrophilic medium for chlorination of deactivated arenes. <i>Applied Catalysis A: General</i> , 2011, 401, 176-181.	2.2	21
4945	Molecular modelling and competition binding study of Br-noscapine and colchicine provide insight into noscapinoidâ€™ tubulin binding site. <i>Journal of Molecular Graphics and Modelling</i> , 2011, 29, 947-955.	1.3	53
4946	Understanding the stability, electronic and molecular structure of some copper(III) complexes containing alkyl and non alkyl ligands: Insights from DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 2627-2634.	0.8	12
4947	Formation, photophysics, and photochemistry of cadmium(II) complexes with 5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin and its octabromo derivative: The effects of bromination and the axial hydroxo ligand. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011, 218, 143-155.	2.0	31
4948	Chemically accurate and computationally-efficient time-dependent density functional theory (TDDFT) modeling of the UV/Vis spectra of Pechmann dyes and related compounds. <i>Procedia Computer Science</i> , 2011, 4, 1157-1166.	1.2	5
4949	¹ H and ¹³ C NMR spectra, structure and physicochemical features of phenyl acridine-9-carboxylates and 10-methyl-9-(phenoxy-carbonyl)acridinium trifluoromethanesulphonates â€™ alkyl substituted in the phenyl fragment. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 78, 401-409.	2.0	12
4950	TD-DFT investigation of triple-stranded helicates with bis(benzene-o-dithiolato) ligands. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 78, 1037-1045.	2.0	4
4951	R-phenyldicarboxyl (R=H, NO ₂ and COOH) modular effect on Ni(II) coordination polymers incorporated with a versatile connector 1H-3-(3-pyridyl)-5-(4-pyridyl)-1,2,4-triazole. <i>Polyhedron</i> , 2011, 30, 1213-1218.	1.0	12

#	ARTICLE	IF	CITATIONS
4952	Anharmonic vibrational spectroscopy and investigation of intramolecular mode couplings in adenine. <i>Vibrational Spectroscopy</i> , 2011, 56, 51-59.	1.2	12
4953	Design of new benzothiadiazole-based linear and star molecules with different functional groups as solar cells materials: A theoretical approach. <i>Solar Energy Materials and Solar Cells</i> , 2011, 95, 1800-1810.	3.0	33
4954	Novel dispirobifluorenes and indeno-spirobifluorenes: syntheses and properties. <i>Tetrahedron</i> , 2011, 67, 1201-1209.	1.0	10
4955	DFT studies of N-alkoxyaminy radicals: ESR parameters, UV-vis absorptions and generations. <i>Tetrahedron</i> , 2011, 67, 2260-2268.	1.0	10
4956	Chiral phosphine-phosphite ligands in the enantioselective 1,4-addition of Grignard reagents to β,β -unsaturated carbonyl compounds. <i>Tetrahedron: Asymmetry</i> , 2011, 22, 887-892.	1.8	52
4957	Trajectory calculations of OH radical- and Cl atom-initiated reaction of glyoxal: atmospheric chemistry of the HC(O)CO radical. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6296.	1.3	16
4958	On the mechanism of the reaction of white phosphorus with silylenes. <i>Dalton Transactions</i> , 2011, 40, 7193.	1.6	11
4959	A DFT Explanation of the Reactivity and Regioselectivity of the Diels-Alder Reactions Between 2,3,4,4a-Tetrahydroquinoline and some Electron-Deficient Dienophiles. <i>Letters in Organic Chemistry</i> , 2011, 8, 119-124.	0.2	0
4960	Synthesis, and Acid-Base and DNA-Binding Properties of a Thiophen-Appended Ruthenium Complex. <i>Australian Journal of Chemistry</i> , 2011, 64, 206.	0.5	12
4961	Thickness dependent structural and electronic properties of CuO grown on SrTiO ₃ (100): a hybrid density functional theory study. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 045004.	0.7	8
4962	Simulations of light induced processes in water based on <i>ab initio</i> path integrals molecular dynamics. II. Photoionization. <i>Journal of Chemical Physics</i> , 2011, 135, 154302.	1.2	26
4963	Cr(CO) ₆ photochemistry: Semi-classical study of UV absorption spectral intensities and dynamics of photodissociation. <i>Journal of Chemical Physics</i> , 2011, 134, 164305.	1.2	28
4964	Chasing charge localization and chemical reactivity following photoionization in liquid water. <i>Journal of Chemical Physics</i> , 2011, 135, 224510.	1.2	90
4965	Flickering dipoles in the gas phase: Structures, internal dynamics, and dipole moments of β -naphthol-H ₂ O in its ground and excited electronic states. <i>Journal of Chemical Physics</i> , 2011, 134, 114304.	1.2	9
4966	Communication: Rationale for a new class of double-hybrid approximations in density-functional theory. <i>Journal of Chemical Physics</i> , 2011, 135, 101102.	1.2	93
4967	Importance of complex orbitals in calculating the self-interaction-corrected ground state of atoms. <i>Physical Review A</i> , 2011, 84, .	1.0	75
4968	Finite-size correction in many-body electronic structure calculations of magnetic systems. <i>Physical Review B</i> , 2011, 84, .	1.1	14
4969	Effect of onsite Coulomb repulsion on thermoelectric properties of full-Heusler compounds with pseudogaps. <i>Physical Review B</i> , 2011, 84, .	1.1	52

#	ARTICLE	IF	CITATIONS
4970	Dinitrogen activation by low-coordinate transition metal complexes. Journal of Coordination Chemistry, 2011, 64, 3123-3135.	0.8	7
4971	Communication: A global hybrid generalized gradient approximation to the exchange-correlation functional that satisfies the second-order density-gradient constraint and has broad applicability in chemistry. Journal of Chemical Physics, 2011, 135, 191102.	1.2	254
4972	Oxygen adsorption at LaSrMnO_3 surfaces: Predictions from first principles. Physical Review B, 2011, 83, .	1.1	32
4973	Modeling the iron oxides and oxyhydroxides for the prediction of environmentally sensitive phase transformations. Physical Review B, 2011, 83, .	1.1	64
4974	Tuning the reactivity of semiconductor surfaces by functionalization with amines of different basicity. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 956-960.	3.3	51
4975	Density functional theory calculations of redox properties of iron-sulphur protein analogues. Molecular Simulation, 2011, 37, 572-590.	0.9	13
4976	CO ₂ adsorption on TiO ₂ (101) anatase: A dispersion-corrected density functional theory study. Journal of Chemical Physics, 2011, 135, 124701.	1.2	119
4977	QSRR Study on GC Retention Time of Volatile Components from Hawthorn Perfume. Advanced Materials Research, 2011, 236-238, 2815-2819.	0.3	1
4978	Pt(II) and Pt(IV) Amido, Aryloxy, and Hydrocarbyl Complexes: Synthesis, Characterization, and Reaction with Dihydrogen and Substrates that Possess C-H Bonds. Inorganic Chemistry, 2011, 50, 4195-4211.	1.9	28
4979	A density functional study on dielectric properties of acrylic acid grafted polypropylene. Journal of Chemical Physics, 2011, 134, 134904.	1.2	7
4980	Isomers of the Cu ₅ cluster: a density function theory study. Chinese Physics B, 2011, 20, 033105.	0.7	0
4986	Tuning the electronic coupling in a low-bandgap donor-acceptor copolymer via the placement of side-chains. Journal of Chemical Physics, 2011, 134, 114901.	1.2	34
4987	Why do disilanes fail to fluoresce?. Collection of Czechoslovak Chemical Communications, 2011, 76, 2085-2116.	1.0	4
4988	NMR in Van Vleck magnetism and intermolecular interactions in molecular crystals and Chevrel phases. Physics-Uspekhi, 2011, 54, 499-517.	0.8	4
4989	Dependence of dispersion coefficients on atomic environment. Journal of Chemical Physics, 2011, 135, 234109.	1.2	31
4990	High-performance computing for materials design to advance energy science. MRS Bulletin, 2011, 36, 169-174.	1.7	15
4991	Quantum-Chemical Ab Initio Calculations on Borabenzene (C ₅ H ₅ B) and its Adducts with Ne, Ar, Kr, and N ₂ . Could Free Borabenzene be Observed in Rare Gas Matrices?. Australian Journal of Chemistry, 2011, 64, 957.	0.5	13
4992	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
4994	Comparing modern density functionals for conjugated polymer band structures: Screened hybrid, Minnesota, and Rung 3.5 approximations. <i>Journal of Chemical Physics</i> , 2011, 134, 184105.	1.2	46
4995	Chemistry of defect induced photoluminescence in chalcopyrites: The case of CuAlS ₂ . <i>Journal of Applied Physics</i> , 2011, 109, .	1.1	35
4996	Correcting model energies by numerically integrating along an adiabatic connection and a link to density functional approximations. <i>Journal of Chemical Physics</i> , 2011, 134, 214108.	1.2	10
4997	Electron transfer dissociation of a melectin peptide: correlating the precursor ion structure with peptide backbone dissociations. <i>Collection of Czechoslovak Chemical Communications</i> , 2011, 76, 295-309.	1.0	7
4998	Computational assessment of the environmental fate, bioaccumulation, and toxicity potential of brominated benzylpolystyrene. <i>Toxicology Mechanisms and Methods</i> , 2011, 21, 183-192.	1.3	6
4999	Improved hybrid functional for solids: The HSEsol functional. <i>Journal of Chemical Physics</i> , 2011, 134, 024116.	1.2	292
5000	Self-consistent, constrained linear-combination-of-atomic-potentials approach to quantum mechanics. <i>Journal of Chemical Physics</i> , 2011, 134, 044122.	1.2	6
5001	Theoretical predictions of red and near-infrared strongly emitting <i>X</i> -annulated rylenes. <i>Journal of Chemical Physics</i> , 2011, 134, 074510.	1.2	20
5002	The large quadrupole of water molecules. <i>Journal of Chemical Physics</i> , 2011, 134, 134501.	1.2	49
5003	Simulations of light induced processes in water based on ab initio path integrals molecular dynamics. I. Photoabsorption. <i>Journal of Chemical Physics</i> , 2011, 135, 154301.	1.2	38
5004	Chemical reactions modulated by mechanical stress: Extended Bell theory. <i>Journal of Chemical Physics</i> , 2011, 135, 164103.	1.2	101
5005	CAN NEUTRAL AND IONIZED POLYCYCLIC AROMATIC HYDROCARBONS BE CARRIERS OF THE ULTRAVIOLET EXTINCTION BUMP AND THE DIFFUSE INTERSTELLAR BANDS?. <i>Astrophysical Journal</i> , 2011, 742, 2.	1.6	57
5006	Tetrahydrofolate Recognition by the Mitochondrial Folate Transporter. <i>Journal of Biological Chemistry</i> , 2011, 286, 31480-31489.	1.6	35
5007	Assessment of correlation energies based on the random-phase approximation. <i>New Journal of Physics</i> , 2012, 14, 043002.	1.2	137
5008	The role of relativity and dispersion controlled inter-chain interaction on the band gap of thiophene, selenophene, and tellurophene oligomers. <i>Journal of Chemical Physics</i> , 2012, 136, 094904.	1.2	22
5009	A Molecular Dynamics (MD) and Quantum Mechanics/Molecular Mechanics (QM/MM) Study on Ornithine Cyclodeaminase (OCD): A Tale of Two Iminiums. <i>International Journal of Molecular Sciences</i> , 2012, 13, 12994-13011.	1.8	13
5010	Non-empirical improvement of PBE and its hybrid PBEO for general description of molecular properties. <i>Journal of Chemical Physics</i> , 2012, 136, 104108.	1.2	78
5011	Regulation of the H4 tail binding and folding landscapes via Lys-16 acetylation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 17857-17862.	3.3	82

#	ARTICLE	IF	CITATIONS
5012	Quantum Monte Carlo for the x-ray absorption spectrum of pyrrole at the nitrogen K-edge. Journal of Chemical Physics, 2012, 136, 144301.	1.2	1
5013	Atomic-scale computer simulation of functional materials: methodologies and applications. , 2012, , 643-662e.		0
5014	Experimental and theoretical investigations on photoabsorption and photoionization of trimethylphosphate in the vacuum-ultraviolet energy range. Journal of Chemical Physics, 2012, 137, 184305.	1.2	7
5015	Computational Investigations on Organic Sensitizers for Dye-Sensitized Solar Cell. Current Organic Synthesis, 2012, 9, 215-232.	0.7	20
5016	Optical response of extended systems from time-dependent Hartree-Fock and time-dependent density-functional theory. Journal of Physics: Conference Series, 2012, 367, 012001.	0.3	12
5017	The dynamics of the C + PH ₃ reaction: A theoretical study. Journal of Chemical Physics, 2012, 137, 014316.	1.2	5
5018	Long-range correlation energies from frequency-dependent weighted exchange-hole dipole polarisabilities. Journal of Chemical Physics, 2012, 136, 014104.	1.2	15
5019	Nuclear spin optical rotation and Faraday effect in gaseous and liquid water. Journal of Chemical Physics, 2012, 136, 184502.	1.2	21
5020	Importance of the correlation contribution for local hybrid functionals: Range separation and self-interaction corrections. Journal of Chemical Physics, 2012, 136, 014111.	1.2	83
5021	Nonspherical model density matrices for Rung 3.5 density functionals. Journal of Chemical Physics, 2012, 136, 024111.	1.2	20
5022	Improved constraint satisfaction in a simple generalized gradient approximation exchange functional. Journal of Chemical Physics, 2012, 136, 144115.	1.2	31
5023	Vibronic coupling in asymmetric bichromophores: Theory and application to diphenylmethane. Journal of Chemical Physics, 2012, 137, 084112.	1.2	24
5024	Nonempirical Rung 3.5 density functionals from the Lieb-Oxford bound. Journal of Chemical Physics, 2012, 137, 224110.	1.2	17
5025	Spin densities from subsystem density-functional theory: Assessment and application to a photosynthetic reaction center complex model. Journal of Chemical Physics, 2012, 136, 194104.	1.2	35
5026	Influence of doping on the photoactive properties of magnetron-sputtered titania coatings: Experimental and theoretical study. Physical Review B, 2012, 86, .	1.1	23
5027	Direct comparison of optimized effective potential and Hartree-Fock self-consistent calculations for jellium slabs. Physical Review B, 2012, 85, .	1.1	11
5028	Electronic structure of CrN: A comparison between different exchange correlation potentials. Physical Review B, 2012, 85, .	1.1	42
5029	Benchmark study for the application of density functional theory to the prediction of octahedral tilting in perovskites. Physical Review B, 2012, 86, .	1.1	28

#	ARTICLE	IF	CITATIONS
5030	Choice of basic variables in current-density-functional theory. <i>Physical Review A</i> , 2012, 86, .	1.0	52
5031	Correlation energies beyond the random-phase approximation: Inhomogeneous Singwi-Tosi-Land-Sjolander functional applied to spherical atoms and ions. <i>Physical Review A</i> , 2012, 85, .	1.0	20
5032	Binding of styrene on silicon (111)-7Å ² surfaces as a model molecular electronics system. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2012, 30, 031401.	0.9	1
5033	Range-separated hybrid exchange-correlation functional analyses of anatase TiO ₂ doped with W, N, S, W/N, or W/S. <i>Physical Review B</i> , 2012, 86, .	1.1	50
5034	Potential energy surface for dissociation including spin-orbit effects. <i>Molecular Physics</i> , 2012, 110, 2599-2609.	0.8	6
5035	Length dependence of frontier orbital alignment in aromatic molecular junctions. <i>Applied Physics Letters</i> , 2012, 101, .	1.5	44
5036	THEORETICAL STUDY ON CUI-CATALYZED LIGAND-FREE N-ARYLATION OF IMIDAZOLE WITH BROMOBENZENE. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 1135-1147.	1.8	9
5037	Band gap engineering of (N, Si)-codoped TiO ₂ from hybrid density functional theory calculations. <i>New Journal of Physics</i> , 2012, 14, 053007.	1.2	26
5038	ATOMIC DIPOLE MOMENT CORRECTED HIRSHFELD POPULATION METHOD. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 163-183.	1.8	384
5039	The effect of the Perdew-Zunger self-interaction correction to density functionals on the energetics of small molecules. <i>Journal of Chemical Physics</i> , 2012, 137, 124102.	1.2	89
5040	Effect of hydrogen bond formation on the elastic molecular scattering: a case study with methanol. <i>Molecular Physics</i> , 2012, 110, 297-306.	0.8	11
5041	Formation energies and the stability of the oxides of K. <i>Molecular Simulation</i> , 2012, 38, 1308-1314.	0.9	6
5042	Hydration and Proton Transfer in 3M ⁺ PEM Ionomers: An Ab Initio Study. <i>Materials Research Society Symposia Proceedings</i> , 2012, 1384, 1.	0.1	1
5043	Comment on "Revised electron affinity of SF ₆ from kinetic data" [J. Chem. Phys. 136, 121102 (2012)]. <i>Journal of Chemical Physics</i> , 2012, 136, 197101.	1.2	13
5044	Applications of Potential Energy Surfaces in the Study of Enzymatic Reactions. <i>Advances in Physical Chemistry</i> , 2012, 2012, 1-15.	2.0	16
5045	Prediction of Thermodynamic and Kinetic Parameters for Interfacial Reactions of the SiO ₂ System by Quantum Chemistry Methods. <i>Soft Materials</i> , 2012, 10, 285-312.	0.8	3
5046	On the accuracy of frozen density embedding calculations with hybrid and orbital-dependent functionals for non-bonded interaction energies. <i>Journal of Chemical Physics</i> , 2012, 137, 014102.	1.2	20
5047	Exploring the competition between localization and delocalization of the neutral soliton defect in polyenyl chains with the orbital optimized second order opposite spin method. <i>Journal of Chemical Physics</i> , 2012, 136, 054113.	1.2	21

#	ARTICLE	IF	CITATIONS
5048	Nuclear spin- ρ spin constants, rotational g factor and susceptibility of sulphur hexafluoride. <i>Molecular Physics</i> , 2012, 110, 2163-2172.	0.8	0
5049	Theoretical Investigation of the Reaction of Yttrium Cation with Acetone. <i>Zeitschrift Fur Physikalische Chemie</i> , 2012, 226, 219-231.	1.4	0
5050	Multiscale, Multiparadigm Modeling for Nanosystems Characterization and Design. <i>The Electrical Engineering Handbook</i> , 2012, , 935-982.	0.2	0
5051	How Does Methanol Assist the Hydrogen Transfer in Pd-catalyzed Cyclocarbonylation of Allylic Alcohols? Insights from a DFT Study. <i>Chemistry Letters</i> , 2012, 41, 693-695.	0.7	1
5052	Effectiveness of Optimizing Geometry for CaMn ₄ O ₅ Cluster at 1.9 Å... Resolved OEC and Proposal for Oxidation Mechanism from S ₀ to S ₃ States. <i>Chemistry Letters</i> , 2012, 41, 18-20.	0.7	13
5053	The pH sensor of the plant K ⁺ -uptake channel KAT1 is built from a sensory cloud rather than from single key amino acids. <i>Biochemical Journal</i> , 2012, 442, 57-63.	1.7	20
5054	Mechanistic Consideration of Asymmetric C-N and C-C Bond Formations with Bifunctional Chiral Ir and Ru Catalysts. <i>Bulletin of the Chemical Society of Japan</i> , 2012, 85, 316-334.	2.0	13
5055	COMPUTATIONAL STUDY OF INTERSTELLAR GLYCINE FORMATION OCCURRING AT RADICAL SURFACES OF WATER-ICE DUST PARTICLES. <i>Astrophysical Journal</i> , 2012, 754, 24.	1.6	51
5056	Platinum(II)-Catalyzed Cyclization Sequence of Aryl Alkynes via C(sp ³)-H Activation: A DFT Study. <i>Journal of Organic Chemistry</i> , 2012, 77, 6076-6086.	1.7	13
5057	Combined Theoretical and Experimental Investigation of the Photodecarboxylation of Nitrophenylacetates and Its Implications for the Design of Improved <i>ortho</i> -Nitrobenzylic Caging Groups. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11846-11862.	1.1	9
5058	Varying the Lewis Base Coordination of the Y ₂ N ₂ Core in the Reduced Dinitrogen Complexes $\{[(\text{Me})_3\text{Si})_2\text{N}_2(\text{L})_2(\text{Y})_2]^{1/4-1/2+} : \text{N}_2\}^{2+}$ (L = Benzonitrile, Pyridines, Triphenylphosphine Oxide, and Trimethylamine <i>N</i> -Oxide). <i>Inorganic Chemistry</i> , 2012, 51, 7867-7874.	1.1	13
5059	Theoretical Kinetic Study of Thermal Decomposition of Cyclohexane. <i>Energy & Fuels</i> , 2012, 26, 2811-2820.	2.5	44
5060	Infinite Copper(II) Coordination Architectures from a Resonative Aminotriazine-Derived Tripodal Ligand: Synthesis, Structures, and Magnetic Properties. <i>Inorganic Chemistry</i> , 2012, 51, 12360-12371.	1.9	10
5061	High pressure ices. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 745-750.	3.3	92
5062	Carbenoid Alkene Insertion Reactions of Oxiranyllithiums. <i>Journal of Organic Chemistry</i> , 2012, 77, 8605-8614.	1.7	7
5063	Improved Mode Assignment for Molecular Crystals Through Anisotropic Terahertz Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10359-10364.	1.1	26
5064	Chiral Interconversions of Pd and/or Au Bis-Metalated [32]Octaphyrins(1,0,1,0,1,0,1,0) Involving Hückel and Möbius Macrocyclic Topologies: A Theoretical Prediction. <i>Journal of Organic Chemistry</i> , 2012, 77, 8124-8130.	1.7	13
5065	Response of Crown Ether Functionalized Polythiophenes to Alkaline Ions. <i>Journal of Physical Chemistry B</i> , 2012, 116, 4575-4583.	1.2	8

#	ARTICLE	IF	CITATIONS
5066	TD-DFT Assessment of Functionals for Optical $\pi \rightarrow \pi^*$ Transitions in Solvated Dyes. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2359-2372.	2.3	403
5067	Design, Synthesis, and Analysis of the Quantitative Structure-Activity Relationships of 4-Phenyl-acyl-substituted 3-(2,5-Dimethylphenyl)-4-hydroxy-1-azaspiro[4.5]dec-3-ene-2,8-dione Derivatives. <i>Journal of Agricultural and Food Chemistry</i> , 2012, 60, 4779-4787.	2.4	11
5068	Spectroscopic and Computational Studies of a Small-Molecule Functional Mimic of Iron Superoxide Dismutase, Iron 2,6-Diacetylpyridinebis(semioxamazine). <i>Inorganic Chemistry</i> , 2012, 51, 12729-12737.	1.9	6
5069	The π -conjugated P-flowers C16(PH)8 and C16(PF)8 are potential materials for organic n-type semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14832.	1.3	23
5070	Vanadocene <i>de Novo</i> : Spectroscopic and Computational Analysis of Bis(η^5 -cyclopentadienyl)vanadium(II). <i>Organometallics</i> , 2012, 31, 8265-8274.	1.1	25
5071	Theoretical assessment of the viability of thermal [2+2] processes for formation of plumisclerin A. <i>Tetrahedron Letters</i> , 2012, 53, 6919-6922.	0.7	12
5072	Pyrene-Fluorene Hybrids Containing Acetylene Linkage as Color-Tunable Emitting Materials for Organic Light-Emitting Diodes. <i>Journal of Organic Chemistry</i> , 2012, 77, 3921-3932.	1.7	91
5073	Understanding Rhodopsin Mutations Linked to the <i>Retinitis pigmentosa</i> Disease: a QM/MM and DFT/MRCI Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1060-1076.	1.2	18
5074	Intramolecular Hydrogen Bonding Plays a Crucial Role in the Photophysics and Photochemistry of the GFP Chromophore. <i>Journal of the American Chemical Society</i> , 2012, 134, 1662-1672.	6.6	200
5075	Structural transitions and transport-half-metallic ferromagnetism in LaMnO_3 at elevated pressure. <i>Physical Review B</i> , 2012, 85, .	1.1	36
5076	Structure of Carboxyl-Acid-Terminated Self-Assembled Monolayers from Molecular Dynamics Simulations and Hybrid Quantum Mechanics-Molecular Mechanics Vibrational Normal-Mode Analysis. <i>Journal of Physical Chemistry C</i> , 2012, 116, 770-782.	1.5	18
5077	Hydrogen bond effects in the vibrational spectra of 1,3-propanediol in acetonitrile: <i>ab initio</i> and experimental study. <i>Journal of Chemical Physics</i> , 2012, 137, 244501.	1.2	10
5078	Configurational Assignment of Cyclic Bisbibenzyls by HPLC-CD and Quantum-Chemical CD Calculations. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 6878-6887.	1.2	13
5079	Perspectives on <i>ab initio</i> molecular simulation of excited-state properties of organic dye molecules in dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12044.	1.3	33
5080	An Efficient One-Pot Three-Component Synthesis of Highly Functionalized Coumarin Fused Indenodihydropyridine and Chromeno[4,3-b]quinoline Derivatives. <i>Heterocycles</i> , 2012, 85, 1629.	0.4	15
5081	Model Iron-Oxo Species and the Oxidation of Imidazole: Insights into the Mechanism of OvoA and EgtB?. <i>Inorganic Chemistry</i> , 2012, 51, 13351-13356.	1.9	36
5082	Precise Identification of the Infrared Bands of the Polycarbonyl Complexes on Ni-MOR Zeolite by $^{12}\text{C}^{16}\text{O}$ - $^{13}\text{C}^{18}\text{O}$ Coadsorption and Computational Modeling. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22823-22831.	1.5	15
5083	Two-Component Relativistic Calculations of Electric-Field Gradients Using Exact Decoupling Methods: Spin-orbit and Picture-Change Effects. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4239-4248.	2.3	62

#	ARTICLE	IF	CITATIONS
5084	Accurate Spin-State Energetics of Transition Metal Complexes. 1. CCSD(T), CASPT2, and DFT Study of $[M(NCH)_6]^{2+}$ (M = Fe, Co). <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4216-4231.	2.3	130
5085	Reliable Quantum Chemical Prediction of the Localized/Delocalized Character of Organic Mixed-Valence Radical Anions. From Continuum Solvent Models to Direct-COSMO-RS. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4189-4203.	2.3	83
5086	Vibrationally Resolved Absorption and Emission Spectra of Dithiophene in the Gas Phase and in Solution by First-Principle Quantum Mechanical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4483-4493.	2.3	66
5087	Hybrid functionals and G_W approximation in the FLAPW method. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 293201.	0.7	33
5088	Combined Spectroscopic/Computational Studies of Vitamin B ₁₂ Precursors: Geometric and Electronic Structures of Cobinamides. <i>Inorganic Chemistry</i> , 2012, 51, 2867-2879.	1.9	26
5089	Electronic properties of lanthanide oxides from the G_W perspective. <i>Physical Review B</i> , 2012, 86, .	1.1	96
5090	Analytical expression for the excited-state force from density-functional perturbation theory. <i>Physical Review A</i> , 2012, 86, .	1.0	3
5091	Modelling peptide-metal dication interactions: formamide-Ca ²⁺ reactions in the gas phase. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7552.	1.5	16
5092	Theoretical study on the hypervalent λ^3 -bromane strategy for Baeyer-Villiger oxidation of benzaldehyde and acetaldehyde: rearrangement mechanism. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 6333.	1.5	6
5093	Vibrational Spectra of Phosphate Ions in Aqueous Solution Probed by First-Principles Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2466-2474.	1.1	41
5094	Changes in Charge Distribution, Molecular Volume, Accessible Surface Area and Electronic Structure along the Reaction Coordinate for a Carbocationic Triple Shift Rearrangement of Relevance to Diterpene Biosynthesis. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8902-8909.	1.1	21
5095	Binding motifs of silver in prion octarepeat model peptides: a joint ion mobility, IR and UV spectroscopies, and theoretical approach. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11433.	1.3	28
5096	Optimized End-Stacking Provides Specificity of N -Methyl Mesoporphyrin IX for Human Telomeric G-Quadruplex DNA. <i>Journal of the American Chemical Society</i> , 2012, 134, 20446-20456.	6.6	176
5097	Short- and long-range binding of Be with Mg in the $X^1\Sigma^+$ ground state and in the $A^1\Pi$ excited state. <i>Journal of Chemical Physics</i> , 2012, 137, 124309.	1.2	4
5098	Nonadiabatic dynamics of a truncated indigo model. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12378.	1.3	45
5099	Efficient Förster Resonance Energy Transfer in 1,2,3-Triazole Linked BODIPY-Zn(II) Meso-tetraphenylporphyrin Donor-Acceptor Arrays. <i>Inorganic Chemistry</i> , 2012, 51, 13114-13122.	1.9	60
5101	The $R_3O^+ \cdot \hat{A} \cdot \hat{A} \cdot H^+$ Hydrogen Bond: Toward a Tetracoordinate Oxadionium(2+) Ion. <i>Journal of the American Chemical Society</i> , 2012, 134, 707-714.	6.6	39
5102	Preparation of phosphorus-doped carbon nanospheres and their electrocatalytic performance for O ₂ reduction. <i>Journal of Natural Gas Chemistry</i> , 2012, 21, 257-264.	1.8	51

#	ARTICLE	IF	CITATIONS
5103	Coordination Effects on Electron Distributions for Rhodium Complexes of the Redox-Active Bis(3,5-di-tert-butyl-2-phenolate)amide Ligand. <i>Inorganic Chemistry</i> , 2012, 51, 12606-12618.	1.9	30
5104	Fine Tuning the Performance of DSSCs by Variation of the "Spacers in Organic Dyes that Contain a 2,7-Diaminofluorene Donor. <i>Chemistry - an Asian Journal</i> , 2012, 7, 2942-2954.	1.7	19
5105	Re-examining the Mechanisms of Competing Pericyclic Reactions of 1,3,7-Octatriene. <i>Chemistry - A European Journal</i> , 2012, 18, 11029-11035.	1.7	6
5106	Can an Amine Be a Stronger Acid than a Carboxylic Acid? The Surprisingly High Acidity of Amine-Borane Complexes. <i>Chemistry - A European Journal</i> , 2012, 18, 15699-15705.	1.7	21
5107	Triguanide Derivatives: Synthesis, Crystal Structure and Evaluation of the Proliferation Effect on Some Tumor Cell Lines. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 6785-6797.	1.2	8
5108	Donor-enhanced bridge effect on the electronic properties of triphenylamine based dyes: density functional theory investigations. <i>Journal of Molecular Modeling</i> , 2012, 18, 3609-3615.	0.8	16
5109	Revisiting caffeate's capabilities as a complexation agent to silver cation in mining processes by means of the dual descriptor—a conceptual DFT approach. <i>Journal of Molecular Modeling</i> , 2012, 18, 4299-4307.	0.8	41
5110	Cluster models of aqueous Na ⁺ and Cl ⁻ in sea water/ice. <i>Journal of Nanoparticle Research</i> , 2012, 14, 1.	0.8	4
5111	Super and hyperhalogen behavior in MgX _n and GdX _n (X = F, BF ₄) clusters. <i>Journal of Nanoparticle Research</i> , 2012, 14, 1.	0.8	19
5112	Spectral character of intermediate state in solid-state photoarrangement of \pm -santonin. <i>Chemical Physics</i> , 2012, 405, 40-45.	0.9	8
5113	Characterization of Ptn (n=2-12) clusters through global reactivity descriptors and vibrational spectroscopy, a theoretical study. <i>Computational Materials Science</i> , 2012, 53, 18-24.	1.4	33
5114	QM/MM studies of cisplatin complexes with DNA dimer and octamer. <i>Computational and Theoretical Chemistry</i> , 2012, 993, 60-65.	1.1	20
5115	Correlating ETD fragment ion intensities with peptide ion conformational and electronic structure. <i>International Journal of Mass Spectrometry</i> , 2012, 330-332, 207-219.	0.7	11
5116	Thermal Stability and Quantum Chemistry Study on Octahydro-2,5-Bis(Nitroimino)imidazo[4,5-d]imidazole. <i>Procedia Engineering</i> , 2012, 45, 558-561.	1.2	2
5117	The effect of 2-aminoquinoline-6-carboxylic acid on the corrosion behavior of mild steel in hydrochloric acid. <i>Journal of the Iranian Chemical Society</i> , 2012, 9, 635-641.	1.2	8
5118	Electronic structure study of the triplet azulene-like molecules. <i>Chemical Physics Letters</i> , 2012, 545, 132-137.	1.2	7
5119	DFT-NEGF study of transport properties and NDR behavior in fused furan and thiophene dimmers. <i>Physica B: Condensed Matter</i> , 2012, 407, 4503-4511.	1.3	6
5120	Which oxidation state is preferable at S0 state in oxygen-evolving complex, Mn ₄ (II, III, IV, IV) or Mn ₄ (III, IV, IV, IV)? <i>Journal of Theoretical Chemistry</i> , 2012, 11, 1078-1084.	1.2	14

#	ARTICLE	IF	CITATIONS
5121	Screened hybrid functional applied to $3d^0$ transition-metal Molecular Redox: Revisiting the Electronic Structures of the Group 9 Metallocorroles. Inorganic Chemistry, 2012, 51, 12473-12482.	1.1	146
5122	DFT Simulation and Vibrational Analysis of the IR and Raman Spectra of a CdSe Quantum Dot Capped by Methylamine and Trimethylphosphine Oxide Ligands. Journal of Physical Chemistry C, 2012, 116, 14674-14681.	1.5	52
5124	Response properties of AgCl and AgBr under an external static electric field: A density functional study. Solid State Sciences, 2012, 14, 1412-1418.	1.5	6
5125	Ultrafast photo-induced charge transfer unveiled by two-dimensional electronic spectroscopy. Journal of Chemical Physics, 2012, 136, 204503.	1.2	49
5126	Synthetic studies towards the mulberry Diels-Alder adducts: H-bond accelerated cycloadditions of chalcones. Organic and Biomolecular Chemistry, 2012, 10, 6010.	1.5	22
5127	On the electronic structure and conflicting d-orbital aromaticity in the $Re_3O_3^{3-}$ cluster. RSC Advances, 2012, 2, 2707.	1.7	16
5128	Magnetic properties of a doped linear polyarylamine bearing a high concentration of coupled spins (S). Journal of Physical Chemistry B, 2012, 116, 14674-14681.	1.3	14
5129	Mechanistic investigation of the iridium-catalysed alkylation of amines with alcohols. Organic and Biomolecular Chemistry, 2012, 10, 2569.	1.5	61
5130	Aquation and dimerization of osmium(ii) anticancer complexes: a density functional theory study. RSC Advances, 2012, 2, 436-446.	1.7	13
5131	Atmospheric hydrocarbonactivation by the hydroxyl radical: a simple yet accurate computational protocol for calculating rate coefficients. Physical Chemistry Chemical Physics, 2012, 14, 184-191.	1.3	20
5132	Toward quantum-dot cellular automata units: thiolated-carbazole linked bisferrocenes. Nanoscale, 2012, 4, 813-823.	2.8	58
5133	Tuning the wavelength of electrochemiluminescence by anodic potential: a design using non-Kekulé-structured iridium-ruthenium luminophores. Dalton Transactions, 2012, 41, 6064.	1.6	41
5134	Vapor Phase Infrared Spectroscopy and Ab Initio Fundamental Anharmonic Frequencies of Ammonia Borane. Journal of Physical Chemistry A, 2012, 116, 3124-3136.	1.1	22
5135	Atmospheric Chemistry of Ethyl Propionate. Journal of Physical Chemistry A, 2012, 116, 5164-5179.	1.1	27
5136	Oxidation Reactions of 2-Thiouracil: A Theoretical and Pulse Radiolysis Study. Journal of Physical Chemistry A, 2012, 116, 10712-10720.	1.1	21
5137	A novel di-compartmental bis-(2-hydroxyisophthalamide) macrocyclic ligand and its mononuclear Cu(ii) and Ni(ii) complexes. Dalton Transactions, 2012, 41, 12457.	1.6	7
5138	Synthesis, experimental and theoretical characterization, and field-effect transistor properties of a new class of dibenzothiophene derivatives: From linear to cyclic architectures. Journal of Materials Chemistry, 2012, 22, 1313-1325.	6.7	41

#	ARTICLE	IF	CITATIONS
5139	Hydrogen-Saturated Silicon Nanowires Heavily Doped with Interstitial and Substitutional Transition Metals. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15713-15722.	1.5	30
5140	Unusually Fast 1,6-H Shifts of Enolic Hydrogens in Peroxy Radicals: Formation of the First-Generation C ₂ and C ₃ Carbonyls in the Oxidation of Isoprene. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6134-6141.	1.1	34
5141	Oxidation Mechanism of Methionine by HO• Radical: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5349-5354.	1.2	9
5142	Critical appraisal of excited state nonadiabatic dynamics simulations of 9 <i>H</i> -adenine. <i>Journal of Chemical Physics</i> , 2012, 137, 22A503.	1.2	102
5143	Synthesis and computational studies of Mg complexes supported by 2,2',6,2'-terpyridine ligands. <i>Dalton Transactions</i> , 2012, 41, 8098.	1.6	5
5144	Experimental and theoretical study of the degradation of malonamide extractant molecules under ionizing radiation. <i>RSC Advances</i> , 2012, 2, 3954.	1.7	6
5145	The effect of hydrogen bond reorganization and equivalent weight on proton transfer in 3M perfluorosulfonic acid ionomers. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 16349.	1.3	24
5146	Fusing cubanes to 1,5-hexadiene. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14756.	1.3	0
5147	Fully relativistic coupled cluster and DFT study of electric field gradients at Hg in 199Hg compounds. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2651.	1.3	31
5148	Structural, spectroscopic and redox properties of a mononuclear CoII thiolate complex – the reactivity toward S-alkylation: an experimental and theoretical study. <i>Dalton Transactions</i> , 2012, 41, 12586.	1.6	9
5149	Hydrogenation of dinitrogen to ammonia in [WF(PH ₂ (CH ₂) ₂ PH ₂) ₂ N ₂] using H ₂ : Insights from DFT calculations. <i>New Journal of Chemistry</i> , 2012, 36, 562.	1.4	14
5150	Isolation and characterization of charge-tagged phenylperoxyl radicals in the gas phase: direct evidence for products and pathways in low temperature benzene oxidation. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 16719.	1.3	33
5151	Assessment of density functional approximations for the hemibonded structure of the water dimer radical cation. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10705.	1.3	41
5152	Equilibrium, photophysical and photochemical examination of anionic lanthanum(III) mono- and bisporphyrins: the effects of the out-of-plane structure. <i>Dalton Transactions</i> , 2012, 41, 13120.	1.6	14
5153	Spectral characteristics, DNA-binding and cytotoxicity of two functional Ru(II) mixed-ligand complexes. <i>Dalton Transactions</i> , 2012, 41, 4575.	1.6	45
5154	Redox and photoisomerization switching of the second-order optical nonlinearity of a tetrathiafulvalene derivative of spiropyran across five states: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 5297.	1.3	23
5155	Structure, electronic configuration, and Mössbauer spectral parameters of an antiferromagnetic Fe ₂ -peroxo intermediate of methane monooxygenase. <i>Dalton Transactions</i> , 2012, 41, 995-1003.	1.6	13
5156	Modulating Nitric Oxide Release by <i>S</i> -Nitrosothiol Photocleavage: Mechanism and Substituent Effects. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7039-7049.	1.1	19

#	ARTICLE	IF	CITATIONS
5157	Theoretical and Experimental Studies of the Spin Trapping of Inorganic Radicals by 5,5-Dimethyl-1-pyrroline <i>N</i> -Oxide (DMPO). 3. Sulfur Dioxide, Sulfito, and Sulfate Radical Anions. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7210-7218.	1.1	145
5158	Energetics and Structure of Uranium(VI) Acetate Complexes in Dimethyl Sulfoxide. <i>Inorganic Chemistry</i> , 2012, 51, 9045-9055.	1.9	45
5159	Electron Configuration and Hydrogen-Bonding Pattern in Several Thymine and Uracil Analogues Studied by ^{14}N NQDR and DFT/QAIM. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8793-8804.	1.2	10
5160	Nature of Isomerism of Solid Isothiourea Salts, Inhibitors of Nitric Oxide Synthases, As Studied by ^{14}N Nuclear Quadrupole Double Resonance, X-ray, and Density Functional Theory/Quantum Theory of Atoms in Molecules. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1445-1463.	1.1	11
5161	Controlling the Formation of Metallic Nanoparticles on Functionalized Silicon Surfaces. <i>Journal of Physical Chemistry C</i> , 2012, 116, 14431-14444.	1.5	21
5162	Electron Attachment to the Cytosine-Centered DNA Single Strands: Does Base Stacking Matter?. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1458-1466.	1.2	11
5163	Kinetics and Mechanisms of the Thermal Decomposition of 2-Methyl-1,3-dioxolane, 2,2-Dimethyl-1,3-dioxolane, and Cyclopentanone Ethylene Ketal in the Gas Phase. Combined Experimental and DFT Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9228-9237.	1.1	8
5164	Magnetic Ordering in Porous Graphenes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 20109-20120.	1.5	8
5165	Fifth Stereoactive Orbital on Silicon: Relaxation of the Lowest Singlet Excited State of Octamethyltrisilane. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10507-10517.	1.1	5
5166	A Recipe for Designing Molecules with Ever-Increasing Electron Affinities. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1469-1474.	1.1	48
5167	Theoretical and Experimental Studies on Circular Dichroism of Carbo[n]helicenes. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7372-7385.	1.1	239
5168	Application of screened hybrid functionals to the bulk transition metals Rh, Pd, and Pt. <i>Physical Review B</i> , 2012, 86, .	1.1	24
5169	Ground and Excited State Properties of New Porphyrin Based Dyads: A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10736-10744.	1.1	21
5170	Gas-Phase Chemical Dynamics Simulations on the Bifurcating Pathway of the Pimaradienyl Cation Rearrangement: Role of Enzymatic Steering in Abietic Acid Biosynthesis. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1212-1222.	2.3	46
5171	Design of Coupled Porphyrin Chromophores with Unusually Large Hyperpolarizabilities. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9724-9733.	1.5	33
5172	Theoretical Investigations on Donor-Acceptor Conjugated Copolymers Based on Naphtho[1,2-c:5,6-c']bis[1,2,5]thiadiazole for Organic Solar Cell Applications. <i>Journal of Physical Chemistry C</i> , 2012, 116, 26154-26161.	1.5	59
5174	Stannylenes: Structures, Electron Affinities, Ionization Energies, and Singlet-Triplet Gaps of Sn_2XY and XSnR_2 Species (X; Y = H, F, Cl, Br, I, and R; $R = \text{C}_2\text{H}_5$) <i>Journal of Physical Chemistry A</i> , 2012, 116, 851-863.	1.9	16
5175	Environmental Sensitivity of Ru(II) Complexes: The Role of the Accessory Ligands. <i>Inorganic Chemistry</i> , 2012, 51, 3355-3365.	1.9	10

#	ARTICLE	IF	CITATIONS
5176	Assessment of Density Functional Theory in Predicting Structures and Free Energies of Reaction of Atmospheric Prenucleation Clusters. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2071-2077.	2.3	168
5177	Tautomerization in the UDP-Galactopyranose Mutase Mechanism: A DFT-Cluster and QM/MM Investigation. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14040-14050.	1.2	14
5178	The Central Role of Gln63 for the Hydrogen Bonding Network and UV-Visible Spectrum of the AppA BLUF Domain. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8064-8073.	1.2	27
5179	Scope of Stereoselective Mn-Mediated Radical Addition to Chiral Hydrazones and Application in a Formal Synthesis of Quinine. <i>Journal of Organic Chemistry</i> , 2012, 77, 3159-3180.	1.7	35
5180	Theoretical Investigation on the Chiral Diamine-Catalyzed Epoxidation of Cyclic Enones: Mechanism and Effects of Cocatalyst. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1251-1260.	1.1	14
5181	Theoretical Investigation of Paramagnetic NMR Shifts in Transition Metal Acetylacetonato Complexes: Analysis of Signs, Magnitudes, and the Role of the Covalency of Ligand-Metal Bonding. <i>Inorganic Chemistry</i> , 2012, 51, 8340-8351.	1.9	56
5182	Factors Governing the Conformational Tendencies of α -Ethylated β -Amino Acids: Chirality and Side-Chain Size Effects. <i>Journal of Physical Chemistry B</i> , 2012, 116, 13297-13307.	1.2	8
5184	Fully Relativistic Calculations of Faraday and Nuclear Spin-Induced Optical Rotation in Xenon. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 91-98.	2.3	23
5185	The Exciton Origin of the Visible Circular Dichroism Spectrum of Bacteriorhodopsin. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6751-6763.	1.2	38
5186	Polarized Raman Spectroscopy of Oligothiophene Crystals To Determine Unit Cell Orientation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6804-6816.	1.1	12
5187	Radical Mechanisms in the Reaction of Organic Halides with Diiminepyridine Cobalt Complexes. <i>Organometallics</i> , 2012, 31, 3958-3971.	1.1	36
5188	Theoretical Investigations on Charge-Transfer Properties of Novel High Mobility n-Channel Organic Semiconductors α -Diazapentacene Derivatives. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22749-22758.	1.5	28
5189	Benchmark Calculations of the Energies for Binding Excess Electrons to Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 893-900.	2.3	39
5190	Computational Evidence for the Catalytic Mechanism of Human Glutathione S-Transferase A3-3: A QM/MM Investigation. <i>ACS Catalysis</i> , 2012, 2, 280-286.	5.5	16
5191	The Effect of Protein Environment on Photoexcitation Properties of Retinal. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2249-2258.	1.2	43
5192	Photoinduced Ligand Exchange and Covalent DNA Binding by Two New Dirhodium Bis-Amidato Complexes. <i>Inorganic Chemistry</i> , 2012, 51, 11882-11890.	1.9	22
5193	Theoretical Elucidation on the Regio-, Diastereo-, and Enantio-Selectivities of Chiral Primary-Tertiary Diamine Catalyst for Asymmetric Direct Aldol Reactions of Aliphatic Ketones. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7082-7088.	1.1	12
5194	Gas-Phase Kinetics Study of Reaction of OH Radical with CH_3NHNH_2 by Second-Order Multireference Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5045-5056.	1.1	13

#	ARTICLE	IF	CITATIONS
5195	Theoretical Study of the O ₂ + Al ₄ (Tetrahedral) System in Its Singlet State and Comparisons with Its Triplet State. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16430-16435.	1.5	5
5196	Theoretical Study of the Switching between H ₄ ckel and M ₂ bius Topologies for Expanded Porphyrins. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24358-24366.	1.5	28
5197	Efficient [WO ₄] ²⁻ -Catalyzed Chemical Fixation of Carbon Dioxide with 2-Aminobenzonitriles to Quinazoline-2,4(1 <i>H</i>),3 <i>H</i> -diones. <i>Inorganic Chemistry</i> , 2012, 51, 13001-13008.	1.9	97
5198	Theoretical Study of Hyperfine Interactions in Small Arsenic-Containing Radicals. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8624-8633.	1.1	5
5199	Theoretical and Experimental Study of Formic Acid Photofragmentation in the Valence Region. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6693-6701.	1.1	7
5200	Regiochemical Effects on Molecular Stability: A Mechanochemical Evaluation of 1,4- and 1,5-Disubstituted Triazoles. <i>Journal of the American Chemical Society</i> , 2012, 134, 9882-9885.	6.6	54
5201	A Comparative Ab Initio Study of the Primary Hydration and Proton Dissociation of Various Imide and Sulfonic Acid Ionomers. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1801-1813.	1.1	30
5202	Dioxomolybdenum(VI) Complexes with Pyrazole Based Aryloxy Ligands: Synthesis, Characterization and Application in Epoxidation of Olefins. <i>Inorganic Chemistry</i> , 2012, 51, 7642-7649.	1.9	52
5203	Calculation of Exchange Coupling Constants in Triply-Bridged Dinuclear Cu(II) Compounds Based on Spin-Flip Constricted Variational Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2268-2277.	1.1	19
5204	In search of the dark state of 5-methyl-2-hydroxypyrimidine using a numerical DFT/MRCI gradient. <i>Molecular Physics</i> , 2012, 110, 2429-2438.	0.8	6
5205	Inner-Sphere Activation, Outer-Sphere Catalysis: Theoretical Study on the Mechanism of Transfer Hydrogenation of Ketones Using Iron(II) PNNP Eneamido Complexes. <i>Organometallics</i> , 2012, 31, 7375-7385.	1.1	79
5206	Energy Densities in the Strong-Interaction Limit of Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3097-3107.	2.3	43
5207	Theoretical Study of the Absorption Spectrum of a Photoisomerizable Iron Complex. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11905-11912.	1.1	6
5208	The One-Electron Reduction Potential of Methionine-Containing Peptides Depends on the Sequence. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9352-9362.	1.2	41
5209	Experimental and Theoretical Charge Density Distribution in a Host-Guest System: Synthetic Terephthaloyl Receptor Complexed to Adipic Acid. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5618-5628.	1.1	8
5210	Complete Reaction Mechanism of Indoleamine 2,3-Dioxygenase as Revealed by QM/MM Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1401-1413.	1.2	68
5211	Mechanistic Insights into the Stepwise Diels-Alder Reaction of 4,6-Dinitrobenzofuroxan. <i>Organic Letters</i> , 2012, 14, 118-121.	2.4	26
5212	Dicyanogermynes: A Tale of Isomers and Interconversions. <i>Inorganic Chemistry</i> , 2012, 51, 12152-12164.	1.9	2

#	ARTICLE	IF	CITATIONS
5213	Temperature Variation of Ultralow Frequency Modes and Mean Square Displacements in Solid Lasamide (Diuretic Drug) Studied by ³⁵ Cl-NQR, X-ray and DFT/QTAIM. Journal of Physical Chemistry A, 2012, 116, 10344-10358.	1.1	4
5214	Potential Energy Surface for Anaerobic Oxidation of Methane via Fumarate Addition. Environmental Science & Technology, 2012, 46, 8244-8252.	4.6	18
5215	Assessment of Theoretical Procedures for Calculating Barrier Heights for a Diverse Set of Water-Catalyzed Proton-Transfer Reactions. Journal of Physical Chemistry A, 2012, 116, 4211-4221.	1.1	92
5216	Theoretical Investigations into C-H Bond Activation Reaction by Nonheme Mn ^{IV} O Complexes: Multistate Reactivity with No Oxygen Rebound. Journal of Physical Chemistry Letters, 2012, 3, 2851-2856.	2.1	77
5217	Implementation of the Solvent Macromolecule Boundary Potential and Application to Model and Realistic Enzyme Systems. Journal of Physical Chemistry B, 2012, 116, 12522-12534.	1.2	14
5218	Trivalent Uranium Complex As a Catalyst to Promote the Functionalization of Carbon Dioxide and Carbon Disulfide: A Computational Mechanistic Study. Journal of Chemical Theory and Computation, 2012, 8, 3605-3617.	2.3	15
5219	Maximally localized Wannier functions in LaMnO ₃ within PBE + <i>U</i> , hybrid functionals and partially self-consistent GW: an efficient route to construct tight-binding parameters for <i>eg</i> -perovskites. Journal of Physics Condensed Matter, 2012, 24, 235602.	0.7	106
5220	Thermal Analysis and Raman Spectra of Different Phases of the Ionic Liquid Butyltrimethylammonium Bis(trifluoromethylsulfonyl)imide. Journal of Physical Chemistry B, 2012, 116, 9238-9245.	1.2	35
5221	Theoretical Prediction of High Pressure Methane Adsorption in Porous Aromatic Frameworks (PAFs). Langmuir, 2012, 28, 14405-14414.	1.6	22
5222	Cold-Surface Photochemistry of Primary and Tertiary Alkyl Nitrites. Journal of Physical Chemistry A, 2012, 116, 6759-6770.	1.1	5
5223	Reductions of Phosphine Oxides and Sulfides by Perchlorosilanes: Evidence for the Involvement of Donor-Stabilized Dichlorosilylene. Journal of Organic Chemistry, 2012, 77, 1-4.	1.7	47
5224	A Theoretical Investigation of Xanthophyll-Protein Hydrogen Bonding in the Photosystem II Antenna. Journal of Physical Chemistry B, 2012, 116, 4310-4318.	1.2	11
5225	C2 Hydroxyl Group Governs the Difference in Hydrolysis Rates of Methyl- ¹³ C-glycero-d-guloseptanoside and Methyl- ¹² C-glycero-d-guloseptanoside. Journal of Organic Chemistry, 2012, 77, 4242-4251.	1.7	14
5226	Theoretical Studies on the Mechanisms and Dynamics of OH Radical with (CH ₃) ₃ COOH and (CH ₃) ₂ CHOOH. Journal of Physical Chemistry A, 2012, 116, 10647-10655.	1.1	6
5227	Unexpected Acidity Enhancement Triggered by AlH ₃ Association to Phosphines. Journal of Physical Chemistry A, 2012, 116, 6950-6954.	1.1	12
5228	Aluminepin: Aluminum Analogues of Borepin and Gallepin. Journal of Organic Chemistry, 2012, 77, 729-732.	1.7	25
5229	Oxidation Mechanism of Aliphatic Ethers: Theoretical Insights on the Main Reaction Channels. Journal of Physical Chemistry A, 2012, 116, 9010-9019.	1.1	14
5230	Role of electronic localization in the phosphorescence of iridium sensitizing dyes. Journal of Chemical Physics, 2012, 137, 154309.	1.2	27

#	ARTICLE	IF	CITATIONS
5231	Nanostructured Diamine-Fullerene Derivatives: Computational Density Functional Theory Study and Experimental Evidence for their Formation via Gas-Phase Functionalization. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1663-1676.	1.1	15
5232	Study of Ion Specific Interactions of Alkali Cations with Dicarboxylate Dianions. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2055-2061.	1.1	24
5233	Synthesis, analysis of spectroscopic and nonlinear optical properties of the novel compound: (S)-N-benzyl-1-phenyl-5-(thiophen-3-yl)-4-pentyn-2-amine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 97, 556-567.	2.0	59
5234	Molecular structure, natural bond analysis, vibrational, and electronic spectra of aspartateguanidoacetatenickel(II), [Ni(Asp)(GAA)]·H ₂ O: DFT quantum mechanical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 97, 1041-1051.	2.0	12
5235	A dinuclear manganese(II) complex {[Na ₂ (H ₂ O) ₄ Mn ₂ (1/4-pmtz) ₄ (NCS) ₂]·xH ₂ O} _n with 5-(pyrimidyl)tetrazolato bridges involved in 1D ladder-like chains: Synthesis, X-ray structure, magnetic properties and DFT calculations. <i>Polyhedron</i> , 2012, 42, 50-56.	1.0	4
5236	Redox coupled-spin crossover in cobalt ^{II} -diketonate complexes: Structural, electrochemical and computational studies. <i>Polyhedron</i> , 2012, 42, 291-301.	1.0	4
5237	An unusual oxidation of the imidazolyl ring in a cobalt terpyridyl complex: Crystal structure and photonuclease activity of the transformed cobalt terpyridyl complex. <i>Polyhedron</i> , 2012, 43, 159-169.	1.0	6
5238	Gold-sulfur bond breaking in Zn(II) tetraphenylporphyrin molecular junctions. <i>Surface Science</i> , 2012, 606, 1412-1415.	0.8	13
5239	Theoretical study on polyaniline gas sensors: Examinations of response mechanism for alcohol. <i>Synthetic Metals</i> , 2012, 162, 862-867.	2.1	27
5240	Novel piperidine-fused benzoxazino- and quinazolinonaphthoxazines synthesis and conformational study. <i>Tetrahedron</i> , 2012, 68, 6284-6288.	1.0	7
5241	Convergence of QM/MM free-energy perturbations based on molecular-mechanics or semiempirical simulations. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12592.	1.3	68
5242	One-pot synthesis of amides by aerobic oxidative coupling of alcohols or aldehydes with amines using supported gold and base as catalysts. <i>Chemical Communications</i> , 2012, 48, 2427.	2.2	96
5243	Mechanism of the Reduction of an Oxidized Glutathione Peroxidase Mimic with Thiols. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5052-5057.	2.3	14
5244	A quantum chemical investigation of the electronic structure of thionine. <i>Photochemical and Photobiological Sciences</i> , 2012, 11, 397-408.	1.6	32
5245	The conformers of 3-fluoroalanine. A theoretical study. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 2084.	1.5	3
5246	How Evenly Can Approximate Density Functionals Treat the Different Multiplicities and Ionization States of 4d Transition Metal Atoms?. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4112-4126.	2.3	37
5247	Electronic excitation spectra of the [Ir(ppy) ₂ (bpy)] ⁺ photosensitizer bound to small silver clusters Ag _n (n = 1-6). <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4977.	1.3	6
5248	Oxidative Aliphatic C-H Fluorination with Fluoride Ion Catalyzed by a Manganese Porphyrin. <i>Science</i> , 2012, 337, 1322-1325.	6.0	478

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5249	Vibrational Circular Dichroism versus Optical Rotation Dispersion and Electronic Circular Dichroism for diastereomers: the stereochemistry of 3-(1-hydroxyethyl)-1-(3-phenylpropanoyl)-azetidin-2-one. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8562.	1.3	30
5250	Overcoming Low Orbital Overlap and Triplet Instability Problems in TDDFT. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9783-9789.	1.1	190
5251	Characterization of a Paramagnetic, Mononuclear Pt(III)-Alkyl Complex Intermediate in Carbon-Halogen Bond Coupling Reactions. <i>Journal of the American Chemical Society</i> , 2012, 134, 15261-15264.	6.6	29
5252	Structure properties relationships of liquid crystal bent core organic semiconductors based on benzo[2,1-b:3,4-b']dithiophene-4,5-dione. <i>Journal of Materials Chemistry</i> , 2012, 22, 23159.	6.7	19
5253	Molecular Modeling to Provide Insight into the Substrate Binding and Catalytic Mechanism of Human Biliverdin-IX α Reductase. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9580-9594.	1.2	26
5254	Theoretical Investigation of the Mechanisms and Stereoselectivities of Reductions of Acyclic Phosphine Oxides and Sulfides by Chlorosilanes. <i>Journal of Organic Chemistry</i> , 2012, 77, 3969-3977.	1.7	43
5255	DFT and Proton Transfer Reactions: A Benchmark Study on Structure and Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3082-3088.	2.3	85
5256	Cobalt in a Bis- β -diketiminato Environment. <i>Inorganic Chemistry</i> , 2012, 51, 11190-11197.	1.9	27
5257	Electronic and Magnetic Properties of Kremer's tris-Hydroxo Bridged Chromium Dimer: A Challenge for DFT. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4915-4921.	2.3	9
5258	Theoretical investigation of rare gas hydride cations: HRgN $_2^+$ (Rg=He, Ar, Kr, and Xe). <i>Journal of Chemical Physics</i> , 2012, 136, 164312.	1.2	21
5259	Mechanism of the N-protecting group dependent annulations of 3-aryloxy alkynyl indoles under gold catalysis: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 4417.	1.5	23
5260	Electronic Structure, Spin-States, and Spin-Crossover Reaction of Heme-Related Fe-Porphyrins: A Theoretical Perspective. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5849-5859.	1.2	102
5261	Imidazole Based Ruthenium(IV) Complexes as Highly Efficient Bifunctional Catalysts for the Redox Isomerization of Allylic Alcohols in Aqueous Medium: Water as Cooperating Ligand. <i>ACS Catalysis</i> , 2012, 2, 2087-2099.	5.5	55
5262	Quantification of Sophisticated Equilibria in the Reaction Pool and Amplifying Catalytic Cycle of the Soai Reaction. <i>ACS Catalysis</i> , 2012, 2, 2137-2149.	5.5	67
5263	Maximally localized Wannier functions: Theory and applications. <i>Reviews of Modern Physics</i> , 2012, 84, 1419-1475.	16.4	2,159
5264	Coordination of Bi $^{3+}$ to metal-free metallothionein: Spectroscopy and density functional calculation of structure, coordination, and electronic excitations. <i>Journal of Inorganic Biochemistry</i> , 2012, 113, 9-14.	1.5	8
5265	Synthesis, crystal structure and redox properties of dihydropyrazole-bridged ferrocene-based derivatives. <i>Journal of Molecular Structure</i> , 2012, 1024, 40-46.	1.8	13
5266	In search of OH \cdots F interactions between 1-methylimidazole and water using a combined computational quantum chemistry and ATR-FTIR spectroscopy approach. <i>Journal of Molecular Structure</i> , 2012, 1026, 78-87.	1.8	6

#	ARTICLE	IF	CITATIONS
5267	Building Hg(II)/Cu(I) multinuclear compounds from mercury bis(phenylselenolate). <i>Journal of Organometallic Chemistry</i> , 2012, 703, 9-15.	0.8	7
5268	Theoretical studies on photo-triggered second-order nonlinear optical switches in a series of polyoxometalate-spiropyran compounds. <i>Journal of Organometallic Chemistry</i> , 2012, 716, 245-251.	0.8	16
5269	A DFT study on the effect of hydrogen in ethylene and propylene polymerization using a Ti-based heterogeneous Ziegler-Natta catalyst. <i>Journal of Organometallic Chemistry</i> , 2012, 719, 74-79.	0.8	45
5270	Strategy for the optical property studies in ultraviolet nonlinear optical crystals from density functional theory. <i>Computational Materials Science</i> , 2012, 60, 99-104.	1.4	71
5271	A QM/MM study on the spinach plastocyanin: Redox properties and absorption spectra. <i>Computational and Theoretical Chemistry</i> , 2012, 990, 119-125.	1.1	55
5272	Electronic structure, bonding, and properties of Sn_mGe_n ($m+n=1/25$) clusters: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2012, 980, 123-132.	1.1	19
5273	DFT modeling of a methane-to-methanol catalytic cycle via Group 6 organometallics: The role of metal in determining the mode of C-H activation. <i>Computational and Theoretical Chemistry</i> , 2012, 980, 133-137.	1.1	12
5274	On the catalytic role of Co^+ in the oxygen transport activation of N_2O by CO . <i>Computational and Theoretical Chemistry</i> , 2012, 982, 2-7.	1.1	4
5275	Reaction of group 16 analogues of ethoxyquin with hydrogen peroxide: A computational study. <i>Computational and Theoretical Chemistry</i> , 2012, 981, 68-72.	1.1	5
5276	Structure and electronic spectral property of coumarin-chalcone hybrids: A comparative study using conventional and long-range corrected hybrid functionals. <i>Computational and Theoretical Chemistry</i> , 2012, 981, 90-99.	1.1	32
5277	Interaction of gold nanoclusters of different size with adenine: A density functional theory study of neutral, anionic and cationic forms of $[\text{adenine}+(\text{Au})_n]^{n=3,6,9,12}$ complexes. <i>Computational and Theoretical Chemistry</i> , 2012, 984, 93-101.	1.1	14
5278	Theoretical investigation of the static (dynamic) polarizability and second hyperpolarizability of DAAD quadrupolar push-pull molecules. A comparison among HF (TD-HF), DFT (TD-B3LYP), and MP2 (TD-MP2) methods. <i>Computational and Theoretical Chemistry</i> , 2012, 985, 72-79.	1.1	24
5279	Differences in hydration between cis- and trans-platin: Quantum insights by ab initio fragment molecular orbital-based molecular dynamics (FMO-MD). <i>Computational and Theoretical Chemistry</i> , 2012, 986, 30-34.	1.1	21
5280	Proton-coupled electron transfer versus hydrogen atom transfer: A density functional reactivity theory characterization. <i>Computational and Theoretical Chemistry</i> , 2012, 988, 13-18.	1.1	4
5281	Density functional theory Raman spectra of cyclic selenium clusters Se_n ($n=5-12$). <i>Computational and Theoretical Chemistry</i> , 2012, 988, 81-85.	1.1	20
5282	Metal salts reduction during parylenes polymerization. <i>Computational and Theoretical Chemistry</i> , 2012, 991, 56-65.	1.1	2
5283	Theoretical studies on the reaction of NO_2 with CO catalyzed by bare Os^+ cations and its kinetic information. <i>Computational and Theoretical Chemistry</i> , 2012, 993, 1-6.	1.1	2
5284	Quantum chemical calculations of the thermal isomerization of 2-methyl-4,5-dihydrofuran. <i>Computational and Theoretical Chemistry</i> , 2012, 993, 53-59.	1.1	1

#	ARTICLE	IF	CITATIONS
5285	Density functional investigation of the molecular structures, vibrational and absorption spectra of metal thiolate complexes, M(SC ₆ H ₅) ₃ (M=As, Sb or Bi). <i>Computational and Theoretical Chemistry</i> , 2012, 994, 91-96.	1.1	6
5286	On the ability of periodic dispersion-corrected DFT calculations to predict molecular crystal polymorphism in para-diiodobenzene. <i>Chemical Physics Letters</i> , 2012, 541, 12-15.	1.2	18
5287	A new meta-GGA exchange functional based on an improved constraint-based GGA. <i>Chemical Physics Letters</i> , 2012, 543, 179-183.	1.2	44
5288	The OH-initiated atmospheric oxidation of divinyl sulfoxide: A theoretical investigation on the reaction mechanism. <i>Chemical Physics Letters</i> , 2012, 543, 61-67.	1.2	2
5289	Jahn-Teller distortion, ferromagnetic coupling, and electron delocalization in a high-spin Fe ²⁺ -Fe bonded dimer. <i>Comptes Rendus Chimie</i> , 2012, 15, 192-201.	0.2	18
5290	Tuning of diglycerol yield and isomer distribution in oligomerization of glycerol supported by DFT-calculations. <i>Catalysis Communications</i> , 2012, 25, 130-135.	1.6	26
5291	Structural, bonding, and magnetic properties of small Fe _n Mox (n, x%6) clusters. <i>Computational Materials Science</i> , 2012, 55, 365-375.	1.4	11
5292	First-principles study of Fe-based superconductors: A comparison of screened hybrid functional with gradient corrected functional. <i>Computational Materials Science</i> , 2012, 55, 284-294.	1.4	4
5293	Electronic band gaps of ternary corundum solid solutions from Fe ₂ O ₃ -Cr ₂ O ₃ -Al ₂ O ₃ system for photocatalytic applications: A theoretical study. <i>Computational Materials Science</i> , 2012, 55, 192-198.	1.4	18
5294	Ultrafast internal conversion in a low band gap polymer for photovoltaics: experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6367.	1.3	43
5295	Insights into the Dual Activation Mechanism Involving Bifunctional Cinchona Alkaloid Thiourea Organocatalysts: An NMR and DFT Study. <i>Journal of Organic Chemistry</i> , 2012, 77, 9813-9825.	1.7	136
5296	Electronic structures and second-order nonlinear optical properties of a series of functionalized Sc ₃ N@Ih ⁻ C ₈₀ derivatives. <i>Computational and Theoretical Chemistry</i> , 2012, 996, 51-56.	1.1	1
5297	Pharmacokinetic Benefits of 3,4-Dimethoxy Substitution of a Phenyl Ring and Design of Isosteres Yielding Orally Available Cathepsin K Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 8827-8837.	2.9	17
5298	Acantholactone, a new manzamine related alkaloid with an unprecedented $\hat{\nu}$ -lactone and $\hat{\mu}$ -lactam ring system. <i>Tetrahedron Letters</i> , 2012, 53, 6329-6331.	0.7	16
5299	Computational elucidation on regio- and stereoselectivity on glycosylation of alcohols by N-Cbz-imino glycal-derived allyl N-nosyl aziridines. <i>Tetrahedron Letters</i> , 2012, 53, 6573-6576.	0.7	1
5300	Dillapiole as Antileishmanial Agent: Discovery, Cytotoxic Activity and Preliminary SAR Studies of Dillapiole Analogues. <i>Archiv Der Pharmazie</i> , 2012, 345, 934-944.	2.1	30
5301	Iridium ⁺ -Catalyzed Allylic Substitutions with Cyclometalated Phosphoramidite Complexes Bearing a Dibenzocyclooctatetraene Ligand: Preparation of (I ⁺ -Allyl)Ir Complexes and Computational and NMR Spectroscopic Studies. <i>Chemistry - A European Journal</i> , 2012, 18, 14314-14328.	1.7	34
5302	Hyperfine Coupling Constants on Inner ⁺ -Sphere Water Molecules of Gd ³⁺ -Based MRI Contrast Agents. <i>ChemPhysChem</i> , 2012, 13, 3640-3650.	1.0	80

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5303	A Photosensitive Liquid Crystal Studied by ^{14}N NMR, ^2H NMR, and DFT Calculations. <i>ChemPhysChem</i> , 2012, 13, 3958-3965.	1.0	11
5304	Microsolvation of morpholine, a bidentate base – the importance of cooperativity. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 1380-1390.	0.9	5
5305	Parameters affecting the luminescence of nanodiamond particles: Quantum chemical calculations. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2012, 209, 1769-1773.	0.8	11
5306	Synthesis and Structure Determination of Two Neutral Cadmium Thiophenolate Clusters. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2012, 638, 2467-2469.	0.6	5
5307	Density functional theory calculation of molecular structures of (5656)macrotetracyclic 3d metal complexes with 4,12-Dithiooxo-1,8-dioxa-3,6,10,13-tetraazacyclotetradecanedione-5,11. <i>Russian Journal of Inorganic Chemistry</i> , 2012, 57, 981-986.	0.3	24
5308	Quantum-chemical calculation of the molecular structures of 3d metal chelates with ligands self-assembled in the M(II)-hydrazinomethane thiohydrazide-acetone systems. <i>Russian Journal of Inorganic Chemistry</i> , 2012, 57, 1100-1106.	0.3	8
5309	Molecular structures of (555)macrotricyclic chelates appearing in 3d-element(ii) ion-hydrazinomethanethioamide-ethanedial systems according to density functional theory calculations. <i>Russian Journal of Inorganic Chemistry</i> , 2012, 57, 1570-1575.	0.3	10
5310	Aza-oxindole synthesis via base promoted Truce – Smiles rearrangement. <i>Chemical Communications</i> , 2012, 48, 10957.	2.2	36
5311	Ab initio quantum chemical and ReaxFF-based study of the intramolecular iminium – enamine conversion in a proline-catalyzed reaction. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	9
5312	Titanium(IV) Trifluoromethyl Complexes: New Perspectives on Bonding from Organometallic Fluorocarbon Chemistry. <i>Organometallics</i> , 2012, 31, 1484-1499.	1.1	37
5313	Driving Unidirectional Molecular Rotary Motors with Visible Light by Intra- And Intermolecular Energy Transfer from Palladium Porphyrin. <i>Journal of the American Chemical Society</i> , 2012, 134, 17613-17619.	6.6	99
5314	Dioxygen Activation by a Non-Heme Iron(II) Complex: Theoretical Study toward Understanding Ferric – Superoxo Complexes. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 915-926.	2.3	65
5315	Why Are $\text{S}_{\text{N}}\text{N}_4$ ($\text{N} = 1-4$) Species – Missing? Answers in a Broader Theoretical Context of Binary – N Compounds. <i>Inorganic Chemistry</i> , 2012, 51, 13321-13327.	1.9	18
5316	Impact of point defects on electronic structure in $\text{Y}_2\text{Ti}_2\text{O}_7$. <i>RSC Advances</i> , 2012, 2, 7235.	1.7	16
5317	Theoretical Modelling of Oxide-Supported Metal Nanoclusters and Nanoalloys. <i>Frontiers of Nanoscience</i> , 2012, , 159-211.	0.3	2
5318	Improving the modified Becke-Johnson exchange potential. <i>Physical Review B</i> , 2012, 85, .	1.1	552
5319	Ruthenium(II) Arene Complexes with Asymmetrical Guanidinate Ligands: Synthesis, Characterization, and Application in the Base-Free Catalytic Isomerization of Allylic Alcohols. <i>Organometallics</i> , 2012, 31, 8301-8311.	1.1	40
5320	Computations of 36 Tautomer/Isomer Equilibria of Different Lactams. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6885-6893.	1.1	11

#	ARTICLE	IF	CITATIONS
5321	A qualitative failure of B3LYP for textbook organic reactions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7170.	1.3	62
5322	Pentacoordinated Organoaluminum Complexes: A Computational Insight. <i>Organometallics</i> , 2012, 31, 8498-8504.	1.1	13
5323	Simulation of NMR Fermi Contact Shifts for Lithium Battery Materials: The Need for an Efficient Hybrid Functional Approach. <i>Journal of Physical Chemistry C</i> , 2012, 116, 17393-17402.	1.5	30
5324	Self-assembling endohedrally doped CdS nanoclusters: new porous solid phases of CdS. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9676.	1.3	12
5325	Towards a Greater Accuracy in DFT Calculations: From GGA to Hybrid Functionals. , 2012, , 3-15.		1
5326	Approaches for Obtaining Accurate Rate Constants for Hydrogen Abstraction by a Chlorine Atom. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3745-3752.	1.1	29
5327	First-Principles Computational Modeling of Fluorescence Resonance Energy Transfer in Co-Sensitized Dye Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2146-2153.	2.1	32
5328	XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12554.	1.3	32
5329	Electric field gradients in Hg compounds: Molecular orbital (MO) analysis and comparison of 4-component and 2-component (ZORA) methods. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 16070.	1.3	13
5330	Hybrid functional calculations of the Al impurity in SiO_2 : Hole localization and electron paramagnetic resonance parameters. <i>Physical Review B</i> , 2012, 85, .	1.1	16
5331	Convergence of Electronic Structure with the Size of the QM Region: Example of QM/MM NMR Shieldings. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2260-2271.	2.3	111
5332	Scalar Relativistic Computations and Localized Orbital Analyses of Nuclear Hyperfine Coupling and Paramagnetic NMR Chemical Shifts. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 598-609.	2.3	87
5333	Radical ions with nearly degenerate ground state: Correlation between the rate of spin-lattice relaxation and the structure of adiabatic potential energy surface. <i>Journal of Chemical Physics</i> , 2012, 137, 104305.	1.2	9
5334	Vapors from Ionic Liquids: Reconciling Simulations with Mass Spectrometric Data. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3435-3441.	2.1	51
5335	Theoretical Prediction of Icosahedral U@C_{20} and Analogous Systems with High HOMO-LUMO Gap. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16716-16725.	1.5	30
5336	Causation in a Cascade: The Origins of Selectivities in Intramolecular Nitrene Cycloadditions. <i>Journal of the American Chemical Society</i> , 2012, 134, 12010-12015.	6.6	19
5337	New Semiconductors Based on 2,2-Ethyne-1,2-diylbis[3-(alk-1-yn-1-yl)thiophene] for Organic Opto-Electronics. <i>Chemistry of Materials</i> , 2012, 24, 2929-2942.	3.2	50
5338	Structural and Photophysical Properties of Visible- and Near-IR-Emitting Tris Lanthanide(III) Complexes Formed with the Enantiomers of N,N' -Bis(1-phenylethyl)-2,6-pyridinedicarboxamide. <i>Inorganic Chemistry</i> , 2012, 51, 647-660.	1.9	70

#	ARTICLE	IF	CITATIONS
5339	Stepwise Diels-Alder: More than Just an Oddity? A Computational Mechanistic Study. <i>Journal of Organic Chemistry</i> , 2012, 77, 6563-6573.	1.7	52
5340	Highly Selective Sorption and Separation of CO ₂ from a Gas Mixture of CO ₂ and CH ₄ at Room Temperature by a Zeolitic Organic-Inorganic Ionic Crystal and Investigation of the Interaction with CO ₂ . <i>Journal of Physical Chemistry C</i> , 2012, 116, 16105-16110.	1.5	35
5341	Linear-Response and Real-Time Time-Dependent Density Functional Theory Studies of Core-Level Near-Edge X-Ray Absorption. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3284-3292.	2.3	192
5342	Higher order alchemical derivatives from coupled perturbed self-consistent field theory. <i>Journal of Chemical Physics</i> , 2012, 136, 034104.	1.2	31
5343	Microwave Magnetic Materials. <i>Handbook of Magnetic Materials</i> , 2012, 20, 1-63.	0.6	8
5345	Modeling the SHG activities of diverse protein crystals. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 1513-1521.	2.5	22
5346	An Atomistic View on Human Hemoglobin Carbon Monoxide Migration Processes. <i>Biophysical Journal</i> , 2012, 102, 887-896.	0.2	43
5347	Protective effect of rutin (vitamin p) against heme oxidation: A quantum mechanical approach. <i>Computational and Theoretical Chemistry</i> , 2012, 996, 28-36.	1.1	16
5348	Density functional theory studies on the mechanism of activation of methane by homonuclear bimetallic Ni-Ni. <i>Computational and Theoretical Chemistry</i> , 2012, 996, 117-124.	1.1	6
5349	A natural bond orbital analysis of carbanions. <i>Computational and Theoretical Chemistry</i> , 2012, 999, 43-47.	1.1	6
5350	Density functional dependence of molecular geometries in lanthanide(III) complexes relevant to bioanalytical and biomedical applications. <i>Computational and Theoretical Chemistry</i> , 2012, 999, 93-104.	1.1	54
5351	Adsorption of CO on pure and mixed clusters of tin and germanium up to five atoms: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2012, 1000, 42-51.	1.1	10
5352	Theoretical investigations of spin-orbit coupling and kinetics in reaction NO ₂ with CO catalyzed by gas phase bare Ir ⁺ . <i>Computational and Theoretical Chemistry</i> , 2012, 1001, 15-19.	1.1	2
5353	Fluorene-based organic dyes containing acetylene linkage for dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2012, 95, 523-533.	2.0	30
5354	Effect of coordinated ligands on antiproliferative activity and DNA cleavage property of three mononuclear Cu(II)-terpyridine complexes. <i>European Journal of Medicinal Chemistry</i> , 2012, 57, 449-458.	2.6	69
5355	Computational model of hydrogen production by Coumarin-dye-sensitized water splitting to absorb the visible light in a local electric field. <i>Energy Conversion and Management</i> , 2012, 62, 154-164.	4.4	13
5356	Dinuclear triple-stranded complexes of ReV with bis(benzene-o-dithiolato) ligands. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 98, 62-69.	2.0	1
5357	Theoretical study of phenylene-thiophene oligomers: Structure-properties relationship. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 99, 126-135.	2.0	13

#	ARTICLE	IF	CITATIONS
5358	Quantum chemistry calculations of branched fluorocarbon systems. <i>Journal of Fluorine Chemistry</i> , 2012, 144, 17-23.	0.9	17
5359	Computational insights on the possibility of tri-coordinated cisplatinated adducts with protein models. <i>Journal of Inorganic Biochemistry</i> , 2012, 117, 230-236.	1.5	4
5360	Anti-inflammatory Active Gold(I) Complexes Involving 6-Substituted-Purine Derivatives. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 4568-4579.	2.9	59
5361	Docking and DFT Studies to explore the Topoisomerase II ATP Pocket employing 3-Substituted 2,6-Piperazindiones for drug design. <i>Molecular Simulation</i> , 2012, 38, 1072-1084.	0.9	13
5362	The Role of Silanols in the Interactions between Methyl <i>tert</i> -Butyl Ether and High-Silica Faujasite Y: An Infrared Spectroscopy and Computational Model Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6943-6952.	1.5	26
5363	Hydration structures of U(III) and U(IV) ions from <i>ab initio</i> molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2012, 137, 074502.	1.2	15
5364	Electronic and magnetic properties of $Ti_{2}O_{3}$, $Cr_{2}O_{3}$, and $Fe_{2}O_{3}$ calculated by the screened exchange hybrid density functional. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 325504.	0.7	82
5365	Formation and Structure of a Platinum(II) Complex Containing Two <i>trans</i> -Nonstabilized Phosphorus Ylide Ligands: Evidence for Reversible Ylide Dissociation. <i>Organometallics</i> , 2012, 31, 3081-3086.	1.1	4
5366	Low-Spin versus High-Spin Ground State in Pseudo-Octahedral Iron Complexes. <i>Inorganic Chemistry</i> , 2012, 51, 6011-6019.	1.9	116
5367	Mild and Efficient Nickel-Catalyzed Heck Reactions with Electron-Rich Olefins. <i>Journal of the American Chemical Society</i> , 2012, 134, 443-452.	6.6	138
5368	Density Functional Theoretical Investigation of Remarkably High Selectivity of the Cs^{+} Ion over the Na^{+} Ion toward Macrocyclic Hybrid Calix-Bis-Crown Ether. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8615-8623.	1.1	40
5369	A FIRST PRINCIPLE ANALYSIS ON THE STRUCTURAL AND PHOTO-INDUCED CHARGE TRANSFER IN RUTHENIUM COMPLEXES OF HEXAAZATRIPHENYLENE. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 895-905.	1.8	5
5370	D-A- π -A Featured Sensitizers Bearing Phthalimide and Benzotriazole as Auxiliary Acceptor: Effect on Absorption and Charge Recombination Dynamics in Dye-Sensitized Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2012, 4, 1822-1830.	4.0	148
5371	Isolation and Characterization of a Class II Mixed-Valence Chromium(I)/(II) Self-Activating Ethylene Trimerization Catalyst. <i>Organometallics</i> , 2012, 31, 486-494.	1.1	25
5372	Exact Kohn-Sham eigenstates versus quasiparticles in simple models of strongly correlated electrons. <i>Physical Review B</i> , 2012, 85, .	1.1	25
5373	Hybrid density functional study of the structural, bonding, and electronic properties of bismuth vanadate. <i>Physical Review B</i> , 2012, 86, .	1.1	55
5374	Quantum Chemistry in Functional Inorganic Materials. <i>Advances in Quantum Chemistry</i> , 2012, 64, 31-81.	0.4	22
5375	Methylation and the system-size effect over the structural, electronic, magnetic (NICS) and reactive properties of pentalene derivatives. <i>Chemical Physics Letters</i> , 2012, 545, 88-94.	1.2	6

#	ARTICLE	IF	CITATIONS
5376	Outer-Sphere Contributions to the Electronic Structure of Type Zero Copper Proteins. <i>Journal of the American Chemical Society</i> , 2012, 134, 8241-8253.	6.6	42
5377	Metal binding selectivity of oxa-aza macrocyclic ligand: a DFT study of first- and second-row transition metal for four coordination systems. <i>Structural Chemistry</i> , 2012, 23, 1539-1545.	1.0	7
5378	Synthesis and Ruthenium Coordination Complexes of the Chelating Phosphine Phosphonium-1-indenylide 1,1-Bis(diphenylphosphino)methane-1-indenylide, 1-C ₉ H ₆ Ph ₂ PCH ₂ PPh ₂ . <i>Organometallics</i> , 2012, 31, 6926-6932.	1.1	5
5379	Range-Separated Exchange Functionals with Slater-Type Functions. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 901-907.	2.3	107
5380	Computational study on the decomposition of tetraeopentyl zirconium for the chemical vapor deposition of zirconium carbide. <i>Korean Journal of Chemical Engineering</i> , 2012, 29, 1438-1443.	1.2	4
5381	Pressure induced insulator/half-metal/metal transition in a strongly correlated p-d electron system. <i>Physical Review B</i> , 2012, 85, .	1.1	10
5382	Quantum Mechanical Study of Pre-Dissociation Enhancement of Linear and Nonlinear Polarizabilities of (TeO ₂) _n Oligomers as a Key to Understanding the Remarkable Dielectric Properties of TeO ₂ Glasses. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9361-9369.	1.1	18
5383	Insufficient Hartree-Fock Exchange in Hybrid DFT Functionals Produces Bent Alkynyl Radical Structures. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 289-293.	2.1	19
5384	MOLECULAR BIOLOGY AT THE QUANTUM LEVEL: CAN MODERN DENSITY FUNCTIONAL THEORY FORGE THE PATH?. <i>Nano LIFE</i> , 2012, 02, 1230006.	0.6	8
5385	Experimental and Theoretical Charge Density Studies of 8-Hydroxyquinoline Cocrystallized with Salicylic Acid. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3420-3427.	1.1	15
5386	Predicting Nuclear Resonance Vibrational Spectra of [Fe(OEP)(NO)]. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 214-223.	2.3	19
5387	Gas-phase reactions of pd with acetone: A theoretical investigation using density functional theory. <i>Russian Journal of Physical Chemistry A</i> , 2012, 86, 1982-1990.	0.1	0
5388	A theoretical study of the reaction of N(4 S) with nitrogen dioxide on the N2O2 potential energy surface. <i>Russian Journal of Physical Chemistry A</i> , 2012, 86, 1438-1446.	0.1	2
5389	Concerted, highly asynchronous, enzyme-catalyzed [4 + 2] cycloaddition in the biosynthesis of spinosyn A; computational evidence. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7503.	1.5	44
5390	Structure-photovoltaic performance relationships for DSSC sensitizers having heterocyclic and benzene spacers. <i>Journal of Materials Chemistry</i> , 2012, 22, 20403.	6.7	22
5391	The Cobalt-Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1870-1894.	2.3	97
5392	New Reaction Model for O=O Bond Formation and O ₂ Evolution Catalyzed by Dinuclear Manganese Complex. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7089-7097.	1.1	16
5393	Geometric parameters of molecular structures of macrotricyclic chelates in MII ion-hydrazinomethane thioamide-butane-2,3-dione ternary systems (M = Co, Ni, Cu) according to the DFT B3LYP quantum chemical calculation. <i>Russian Chemical Bulletin</i> , 2012, 61, 1531-1535.	0.4	5

#	ARTICLE	IF	CITATIONS
5394	Computational study on the multi-channel mechanism of disulfur and ozone reaction. <i>Structural Chemistry</i> , 2012, 23, 1599-1607.	1.0	3
5395	Vibrational Probes and Determinants of the $S = 0 \leftrightarrow S = 2$ Spin Crossover in Five-Coordinate $[\text{Fe}(\text{TPP})(\text{CN})]^{+}$. <i>Inorganic Chemistry</i> , 2012, 51, 11769-11778.	1.9	13
5396	Electronic Structure of Ytterbium Bis-indenyl and -cyclopentadienyl λ^2 -Diimine Complexes: A DFT and MS-CASPT2 Investigation. <i>Organometallics</i> , 2012, 31, 4693-4700.	1.1	11
5397	Modulating the Strength of Hydrogen Bonds through Beryllium Bonds. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2293-2300.	2.3	81
5398	Assigning Structures to Gas-Phase Peptide Cations and Cation-Radicals. An Infrared Multiphoton Dissociation, Ion Mobility, Electron Transfer, and Computational Study of a Histidine Peptide Ion. <i>Journal of Physical Chemistry B</i> , 2012, 116, 3445-3456.	1.2	47
5399	Outer-Sphere Coordination Chemistry: Amido-Ammonium Ligands as Highly Selective Tetrachloridozinc(II)ate Extractants. <i>Inorganic Chemistry</i> , 2012, 51, 12805-12819.	1.9	35
5400	GaMnAs: Position of Mn- d levels and majority spin band gap predicted from GGA-1/2 calculations. <i>Applied Physics Letters</i> , 2012, 100, .	1.5	26
5401	Mechanism of the Acid-Promoted Intramolecular Schmidt Reaction: Theoretical Assessment of the Importance of Lone Pair-Cation, Cation- π , and Steric Effects in Controlling Regioselectivity. <i>Journal of Organic Chemistry</i> , 2012, 77, 640-647.	1.7	41
5402	Fundamentals of Time-Dependent Density Functional Theory. <i>Lecture Notes in Physics</i> , 2012, , .	0.3	370
5403	Reversible Deprotonation and Protonation Behaviors of a Tetra-Protonated λ^3 -Keggin Silicodcatungstate. <i>Inorganic Chemistry</i> , 2012, 51, 7932-7939.	1.9	26
5404	Cruciforms TM Polarized Emission Confirms Disjoint Molecular Orbitals and Excited States. <i>Organic Letters</i> , 2012, 14, 1000-1003.	2.4	15
5405	Multi-decker tricarbonyl-bridged sandwich complexes of transition metals: structure, stability and electron-counting rules. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14803.	1.3	9
5406	Explicitly correlated benchmark calculations on C_8H_8 isomer energy separations: how accurate are DFT, double-hybrid, and composite <i>ab initio</i> procedures?. <i>Molecular Physics</i> , 2012, 110, 2477-2491.	0.8	63
5407	Kinetics of 1,5-Hydrogen Migration in Alkyl Radical Reaction Class. <i>Journal of Physical Chemistry A</i> , 2012, 116, 242-254.	1.1	14
5408	Improved semiconductor lattice parameters and band gaps from a middle-range screened hybrid exchange functional. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 145504.	0.7	72
5409	How to achieve maximum charge carrier loading on heteroatom-substituted graphene nanoribbon edges: density functional theory study. <i>Journal of Materials Chemistry</i> , 2012, 22, 13751.	6.7	22
5410	Radical Cleavage of Al-C Bonds Promoted by Phenazine: From Noninnocent Ligand to Radical Abstractor. <i>Organometallics</i> , 2012, 31, 7011-7019.	1.1	10
5411	Comparative parametric method 6 (PM6) and Recife model 1 (RM1) study of <i>trans</i> -stilbene. <i>Molecular Simulation</i> , 2012, 38, 1-7.	0.9	7

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5412	In Silico Strategies Toward Enzyme Function and Dynamics. <i>Advances in Protein Chemistry and Structural Biology</i> , 2012, 87, 249-292.	1.0	3
5413	Electrochemical antioxidant detection technique based on guanine-bonded graphene and magnetic nanoparticles composite materials. <i>Analyst, The</i> , 2012, 137, 4318.	1.7	13
5414	Theoretical design of the biradical character in 1,3-diphosphacyclobutenediyl and homologous structures. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2015.	1.3	22
5415	Why calcium inhibits magnesium-dependent enzyme phosphoserine phosphatase? A theoretical study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	8
5417	Visible Light Switching of a BF ₂ -Coordinated Azo Compound. <i>Journal of the American Chemical Society</i> , 2012, 134, 15221-15224.	6.6	209
5418	Palladium(II) Containing \hat{I}^3 -Keggin Silicodecatungstate That Efficiently Catalyzes Hydration of Nitriles. <i>Journal of the American Chemical Society</i> , 2012, 134, 6425-6433.	6.6	129
5419	Water Absorbed by Polyaniline Emeraldine Tends to Organize, Forming Nanodrops. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7342-7350.	1.2	16
5420	Mechanistic Insight into the Formal [1,3]-Migration in the Thermal Claisen Rearrangement. <i>Journal of Organic Chemistry</i> , 2012, 77, 10856-10869.	1.7	46
5421	Structural optimization of molecular clusters with density functional theory combined with basin hopping. <i>Journal of Chemical Physics</i> , 2012, 137, 134106.	1.2	45
5422	Laser pulse ionization of fixed-in-space H ₂ O. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2012, 45, 194009.	0.6	5
5423	Theoretical Mn K-edge XANES for Li ₂ MnO ₃ : DFT + <i>U</i> study. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2012, 20, 045006.	0.8	10
5424	Cinnamic Acid Derivatives Acting against <i>Aspergillus</i> Fungi. <i>Taq Polymerase I a Potential Molecular Target</i> . <i>Natural Product Communications</i> , 2012, 7, 1934578X1200701.	0.2	0
5425	Estimating reaction constants by ab initio molecular modeling: a study on the oxidation of phenol to catechol and hydroquinone in advanced oxidation processes. <i>Brazilian Journal of Chemical Engineering</i> , 2012, 29, 113-120.	0.7	8
5426	Coupled-cluster, Møller Plesset (MP2), density fitted local MP2, and density functional theory examination of the energetic and structural features of hydrophobic solvation: Water and pentane. <i>Journal of Chemical Physics</i> , 2012, 136, 054305.	1.2	8
5427	Spectrophotometric investigations and computational calculations of prototropic tautomerism and acid-base properties of some new azo dyes. <i>Dyes and Pigments</i> , 2012, 92, 705-713.	2.0	27
5428	Study on the interaction of Basic Violet 2 with hydroxypropyl- \hat{I}^2 -cyclodextrin. <i>Dyes and Pigments</i> , 2012, 92, 758-765.	2.0	5
5429	Theoretical study on photophysical properties of novel bis(BF ₂) ₂ -bipyrrins dyes: Effect of variation in monomer structure. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 440-452.	1.0	9
5430	Theoretical study on charge transport of quinacridone polymorphs. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 740-746.	1.0	10

#	ARTICLE	IF	CITATIONS
5431	Evaluation of DFT methods to study reactions of benzene with OH radical. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1879-1886.	1.0	13
5432	DFT studies of homogeneous catalysis in the gas phase: Dehydration kinetics of several tertiary alcohols with hydrogen chloride. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 78-88.	1.0	4
5433	Electronic structures of the Cu ₂ S ₂ core of the Cu _A site in cytochrome <i>c</i> oxidase and nitrous oxide reductase. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 208-218.	1.0	7
5434	Ni ₂ H and Ni ₂ Cl homolytic bond dissociation energies and radical stabilization energies: An assessment of theoretical procedures through comparison with benchmark-quality W2w data. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1862-1878.	1.0	46
5435	Analysis of cipadesin limonoids from <i>Cipadessa cinerascens</i> using electrospray ionization quadrupole time-of-flight tandem mass spectrometry and quantum chemical calculations. <i>Rapid Communications in Mass Spectrometry</i> , 2012, 26, 563-571.	0.7	11
5436	A computational exploration of the mechanisms for the acid-catalytic urea-formaldehyde reaction: new insight into the old topic. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 118-125.	0.9	14
5437	Spin-component-scaled electron correlation methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 886-906.	6.2	197
5438	Recent trends in conformational analysis. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 613-641.	6.2	65
5439	Infrared spectra of charge-solvated versus salt-bridge conformations of glycine, serine, and cysteine-Ca ²⁺ complexes. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2126-2134.	1.0	9
5440	The Importance of the DFT method on the computation of the second hyperpolarizability of semiconductor clusters of increasing size: A critical analysis on prolate aluminum phosphide clusters. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2115-2125.	1.0	17
5441	Basis set and functional effects on excited-state properties: Three bicyclic chromogens as working examples. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2135-2141.	1.0	36
5442	Nonharmonic vibrational effects in HgClOH: An MP2 Born-Oppenheimer molecular dynamics study. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3484-3489.	1.0	7
5443	A material design on new sodium ion conductor for sodium-sulfur battery. I. NaAlO(CN) ₂ and Na _x Al _{1-x/3} (CN) ₃ perovskite. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3777-3781.	1.0	9
5444	Laplacian-based models for the exchange energy. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3796-3806.	1.0	20
5445	Reaction mechanism of hydrogenation and direct desulfurization routes of dibenzothiophene-like compounds: A density functional theory study. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3599-3605.	1.0	15
5446	On the energetics of homolytic and heterolytic OH bond cleavage in flavonoids. <i>Computational and Theoretical Chemistry</i> , 2012, 991, 192-200.	1.1	61
5447	A Benchmark Quantum Monte Carlo Study of Molecular Crystal Polymorphism: A Challenging Case for Density-Functional Theory. <i>ACS Symposium Series</i> , 2012, , 101-117.	0.5	7
5448	Surface Acoustic Wave Nebulization Produces Ions with Lower Internal Energy than Electrospray Ionization. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 1062-1070.	1.2	53

#	ARTICLE	IF	CITATIONS
5449	Towards nano-organic chemistry: perspectives for a bottom-up approach to the synthesis of low-dimensional carbon nanostructures. <i>Nanoscale</i> , 2012, 4, 369-379.	2.8	27
5450	Beyond a Single Solvated Electron: Hybrid Quantum Monte Carlo and Molecular Mechanics Approach. <i>ACS Symposium Series</i> , 2012, , 201-206.	0.5	0
5451	Why a Proximity-Induced Diels-Alder Reaction Is So Fast. <i>Organic Letters</i> , 2012, 14, 3016-3019.	2.4	26
5452	Reverse Cope Elimination of Hydroxylamines and Alkenes or Alkynes: Theoretical Investigation of Tether Length and Substituent Effects. <i>Journal of the American Chemical Society</i> , 2012, 134, 2434-2441.	6.6	67
5453	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1515-1531.	2.3	765
5454	Improved Treatment of Surrounding Effects: UV/vis Absorption Properties of a Solvated Ru(II) Complex. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1536-1541.	2.3	47
5455	Unraveling the Electronic Structures of Low-Valent Naphthalene and Anthracene Iron Complexes: X-ray, Spectroscopic, and Density Functional Theory Studies. <i>Inorganic Chemistry</i> , 2012, 51, 6719-6730.	1.9	34
5456	Conformations and Fluorescence of Encapsulated Stilbene. <i>Journal of the American Chemical Society</i> , 2012, 134, 4346-4354.	6.6	40
5457	Chitosan-coated anisotropic silver nanoparticles as a SERS substrate for single-molecule detection. <i>Nanotechnology</i> , 2012, 23, 055501.	1.3	97
5458	Theoretical and experimental investigation on the electronic properties of the shuttlecock shaped and the double-decker structured metal phthalocyanines, MPc and M(Pc) ₂ (M = Sn and Pb). <i>Dalton Transactions</i> , 2012, 41, 7141.	1.6	14
5459	Challenges for Density Functional Theory. <i>Chemical Reviews</i> , 2012, 112, 289-320.	23.0	1,869
5460	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 233202.	0.7	181
5461	A Synthetic and Mechanistic Investigation of the Chromium Tricarbonyl-Mediated Masamune-Bergman Cyclization. Direct Observation of a Ground-State Triplet <i>p</i> -Benzyne Biradical. <i>Organometallics</i> , 2012, 31, 5396-5404.	1.1	16
5462	End-Group-Induced Charge Transfer in Molecular Junctions: Effect on Electronic-Structure and Thermopower. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1962-1967.	2.1	57
5463	Magnetic properties of Co ₂ C and Co ₃ C nanoparticles and their assemblies. <i>Applied Physics Letters</i> , 2012, 101, .	1.5	64
5464	Chapter 2. Transition Metal Systems. <i>RSC Drug Discovery Series</i> , 2012, , 27-55.	0.2	2
5465	Series of New D-A- π -A Organic Broadly Absorbing Sensitizers Containing Isoindigo Unit for Highly Efficient Dye-Sensitized Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2012, 4, 4215-4224.	4.0	124
5466	Water adsorption on rutile TiO ₂ for applications in solar hydrogen production: A systematic hybrid-exchange density functional study. <i>Physical Review B</i> , 2012, 86, .	1.1	29

#	ARTICLE	IF	CITATIONS
5467	Resolution of identity approach for the Kohn-Sham correlation energy within the exact-exchange random-phase approximation. <i>Journal of Chemical Physics</i> , 2012, 136, 134102.	1.2	52
5468	Revealing the true crystal structure of l-phenylalanine using solid-state density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1113-1116.	1.3	32
5469	Mechanistic Study of Oxy Insertion into Nickel–Carbon Bonds with Nitrous Oxide. <i>Organometallics</i> , 2012, 31, 4998-5004.	1.1	28
5470	Stable Alkanes Containing Very Long Carbon–Carbon Bonds. <i>Journal of the American Chemical Society</i> , 2012, 134, 13641-13650.	6.6	181
5471	The mechanism of hexamethylenetetramine (HMT) formation in the solid state at low temperature. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12309.	1.3	52
5472	High Kinetic Stability of HXeBr upon Interaction with Carbon Dioxide: HXeBr·CO ₂ Complex in a Xenon Matrix and HXeBr in a Carbon Dioxide Matrix. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4510-4517.	1.1	32
5473	Exploring new ¹²⁹ Xe chemical shift ranges in HXeY compounds: hydrogen more relativistic than xenon. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10944.	1.3	32
5474	Benchmarking the performance of time-dependent density functional methods. <i>Journal of Chemical Physics</i> , 2012, 136, 104101.	1.2	295
5475	Dyotropic Rearrangements of Fused Tricyclic β -Lactones: Application to the Synthesis of (α^*)-Curcumanolide A and (α^*)-Curcumalactone. <i>Journal of the American Chemical Society</i> , 2012, 134, 13348-13356.	6.6	74
5476	The effect of conjugated spacer on novel carbazole derivatives for dye-sensitized solar cells: Density functional theory/time-dependent density functional theory study. <i>Journal of Computational Chemistry</i> , 2012, 33, 1517-1523.	1.5	28
5477	The electronic spectra and the H-bonding pattern of the sulfur and selenium substituted guanines. <i>Journal of Computational Chemistry</i> , 2012, 33, 1587-1593.	1.5	19
5478	Computational design of improved two-photon active caging compounds based on nitrodibenzofuran. <i>Journal of Computational Chemistry</i> , 2012, 33, 1797-1805.	1.5	11
5479	Metabolic-intermediate complex formation with cytochrome P450: Theoretical studies in elucidating the reaction pathway for the generation of reactive nitroso intermediate. <i>Journal of Computational Chemistry</i> , 2012, 33, 1740-1747.	1.5	30
5480	Kinetics for the hydrogen abstraction of CH ₄ with NO ₂ . <i>Journal of Computational Chemistry</i> , 2012, 33, 1870-1879.	1.5	2
5481	An electronic structure theory investigation of the physical chemistry of the intermolecular complexes of cyclopropenylidene with hydrogen halides. <i>Journal of Computational Chemistry</i> , 2012, 33, 2073-2082.	1.5	11
5482	Probing the electronic structure, chemical bonding, and excitation spectra of [CuE] ⁺⁰ (E = 14 group element) diatomics employing DFT and <i>ab initio</i> methods. <i>Journal of Computational Chemistry</i> , 2012, 33, 2318-2331.	1.5	6
5483	Fragmentation of oxime and silyl oxime ether odd-electron positive ions by the McLafferty rearrangement: new insights on structural factors that promote β , β fragmentation. <i>Journal of Mass Spectrometry</i> , 2012, 47, 676-686.	0.7	11
5484	Direct dynamics study of the hydrogen abstraction reaction of CF ₃ CH ₂ Cl + Cl \rightarrow CF ₃ CHCl + HCl. <i>International Journal of Chemical Kinetics</i> , 2012, 44, 661-667.	1.0	5

#	ARTICLE	IF	CITATIONS
5485	Conformations and intermolecular interactions pattern in solid chloroxylenol and triclosan (API of Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 DFT/QTAIM study. <i>Magnetic Resonance in Chemistry</i> , 2012, 50, 89-105.	1.1	12
5486	Steric and Electronic Influences on the Structures of Peroxomanganese(III) Complexes Supported by Tetradentate Ligands. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 1598-1608.	1.0	23
5487	Copper Complexes with a Hybrid Scorpionate Ligand Containing Pyridazine-3-thione. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 4701-4707.	1.0	20
5488	A Combined Experimental and Computational Study of the Magnetic Superexchange within a Triangular ($\sqrt{3}$ -O)-Pyrazolato-Fe(III) Complex. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 3500-3506.	1.0	15
5489	[4+2] Cycloadditions of 3,4,5,6-tetrahydro-1,2,4-triazole-3-thione and 1,3-butadienes: Synthesis of 3,4,5,6-tetrahydro-1,2,4-triazole-3-thione derivatives. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 2152-2160.	1.2	39
5490	Mechanistic Insight into the Nickel-Catalyzed Intermolecular [3+2+2] Cocyclization of Ethyl Cyclopropylideneacetate with Alkynes: DFT Calculations. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 3911-3915.	1.2	13
5491	Assessment of <i>ab initio</i> MP2 and density functionals for characterizing the potential energy profiles of the S_N2 reactions at N center. <i>Journal of Computational Chemistry</i> , 2012, 33, 1347-1352.	1.5	13
5492	Photoelectron spectroscopy and density functional calculations of $CuSi_n^+$ ($n = 4-18$) clusters. <i>Journal of Chemical Physics</i> , 2012, 136, 104308.	1.2	52
5493	First Principles Design of Ionomers for Facile Ion Transport. <i>ACS Symposium Series</i> , 2012, , 19-44.	0.5	6
5494	Key Mechanistic Features of Enantioselective C-H Bond Activation Reactions Catalyzed by [(Chiral) Tj ETQq1 1 0.784314 rgBT /Overlock 159 2012, 134, 1690-1698.	6.6	159
5495	Intrinsic Metallic and Semiconducting Cubic Boron Nitride Nanofilms. <i>Nano Letters</i> , 2012, 12, 3650-3655.	4.5	42
5496	An Active Site Water Broadens Substrate Specificity in <i>S</i> -Ribosylhomocysteine (LuxS): A Docking, MD, and QM/MM Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8916-8929.	1.2	10
5497	Revisiting [PtCl ₂ (<i>cis</i> -1,4-DACH)]: An Underestimated Antitumor Drug with Potential Application to the Treatment of Oxaliplatin-Refractory Colorectal Cancer. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 7182-7192.	2.9	65
5498	Enantioselective Synthesis of Isoxazolines by 1,3-Dipolar Cycloadditions of Nitrones to Alkynes Catalyzed by Fluorodiphenylmethylpyrrolidines. <i>Advanced Synthesis and Catalysis</i> , 2012, 354, 1665-1671.	2.1	46
5501	Arylsulfonylacetylenes as Alkynylating Reagents of C-H Bonds Activated with Lithium Bases. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 2712-2716.	7.2	56
5502	Aromatic \rightarrow Antiaromatic Switching in Triply Linked Porphyrin Bis(rhodium(I)) Hexaphyrin Hybrids. <i>Chemistry - an Asian Journal</i> , 2012, 7, 889-893.	1.7	30
5503	Effects of ring contraction on the conformational preferences of β -substituted proline analogs. <i>Biopolymers</i> , 2012, 98, 98-110.	1.2	6
5504	Transmetalation Versus β -Hydride Elimination: The Role of 1,4-Benzoquinone in Chelation-Controlled Arylation Reactions with Arylboronic Acids. <i>Chemistry - A European Journal</i> , 2012, 18, 4714-4722.	1.7	39

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5505	Highly Efficient Redox Isomerisation of Allylic Alcohols Catalysed by Pyrazole-Based Ruthenium(IV) Complexes in Water: Mechanisms of Bifunctional Catalysis in Water. <i>Chemistry - A European Journal</i> , 2012, 18, 7749-7765.	1.7	68
5506	Silicon-Containing Formal 4-Electron Four-Membered Ring Systems: Antiaromatic, Aromatic, or Nonaromatic?. <i>Chemistry - A European Journal</i> , 2012, 18, 7516-7524.	1.7	51
5507	Constructing Organic D-A- π -A-Featured Sensitizers with a Quinoxaline Unit for High-Efficiency Solar Cells: The Effect of an Auxiliary Acceptor on the Absorption and the Energy Level Alignment. <i>Chemistry - A European Journal</i> , 2012, 18, 8190-8200.	1.7	171
5508	Design and Function of Pre-organised Outer-Sphere Amidopyridyl Extractants for Zinc(II) and Cobalt(II) Chlorometallates: The Role of C-H Hydrogen Bonds. <i>Chemistry - A European Journal</i> , 2012, 18, 7715-7728.	1.7	28
5509	Metal-Ligand Cooperation in Catalytic Intramolecular Hydroamination: A Computational Study of Iridium-Pyrazolato Cooperative Activation of Aminoalkenes. <i>Chemistry - A European Journal</i> , 2012, 18, 7248-7262.	1.7	25
5510	Correlating DFT-Calculated Energy Barriers to Experiments in Nonheme Octahedral Fe ^{IV} O Species. <i>Chemistry - A European Journal</i> , 2012, 18, 10444-10453.	1.7	24
5511	How Is Methane Formed and Oxidized Reversibly When Catalyzed by Ni-Containing Methyl-Coenzyme M Reductase?. <i>Chemistry - A European Journal</i> , 2012, 18, 6309-6315.	1.7	45
5512	A Density Functional Theory Investigation of the Cobalt-Mediated \hat{I}^{5+} -Pentadienyl/Alkyne [5+2] Cycloaddition Reaction: Mechanistic Insight and Substituent Effects. <i>Chemistry - A European Journal</i> , 2012, 18, 9894-9900.	1.7	9
5513	Viability of M ⁿ -Porphyrin Topologies in [26]- and [28]Hexaphyrins. <i>Chemistry - A European Journal</i> , 2012, 18, 10916-10928.	1.7	48
5514	Expanding the Scope of Arylsulfonylacetylenes as Alkynylating Reagents and Mechanistic Insights in the Formation of Csp ² -Csp and Csp ³ -Csp Bonds from Organolithiums. <i>Chemistry - A European Journal</i> , 2012, 18, 8414-8422.	1.7	42
5515	Mechanism of the Cycloaddition of Carbon Dioxide and Epoxides Catalyzed by Cobalt-Substituted 12-Tungstenphosphate. <i>Chemistry - A European Journal</i> , 2012, 18, 9870-9876.	1.7	56
5516	Origin of Selectivity of Tsuji-Trost Allylic Alkylation of Lactones: Highly Ordered Transition States with Lithium-Containing Enolates. <i>Chemistry - A European Journal</i> , 2012, 18, 10408-10418.	1.7	16
5517	Glycine in 1-Butyl-3-Methylimidazolium Acetate and Trifluoroacetate Ionic Liquids: Effect of Fluorination and Hydrogen Bonding. <i>ChemPhysChem</i> , 2012, 13, 1753-1763.	1.0	18
5518	Properties of Oligothiophene Dendrimers as a Function of Molecular Architecture and Generation Number. <i>ChemPhysChem</i> , 2012, 13, 1354-1362.	1.0	4
5519	Analysis of Nascent Rotational Energy Distributions and Reaction Mechanisms of the Gas-Phase Radical-Radical Reaction O(³ P) + (CH ₃) ₂ CH-C ₃ H ₆ + OH. <i>ChemPhysChem</i> , 2012, 13, 1289-1296.	1.0	5
5520	On the Origin of the Enhanced Acidity of Chalcocyclopentadienes (Cyclopentadiene Chalcogenols) in the Gas Phase. <i>ChemPhysChem</i> , 2012, 13, 1167-1172.	1.0	3
5521	Acene-Modified Triphenylamine Dyes for Dye-Sensitized Solar Cells: A Computational Study. <i>ChemPhysChem</i> , 2012, 13, 2051-2060.	1.0	114
5522	Spiral Intramolecular Charge Transfer and Large First Hyperpolarizability in M ⁿ -Porphyrin Cyclacenes: New Insight into the Localized π Electrons. <i>ChemPhysChem</i> , 2012, 13, 2349-2353.	1.0	23

#	ARTICLE	IF	CITATIONS
5523	Aggregation and Solvation of Chiral N,P-A Amide Ligands in Coordinating Solvents: A Computational and NMR Spectroscopic Study. <i>ChemPlusChem</i> , 2012, 77, 799-806.	1.3	11
5524	Interactions of Electrons with Bare and Hydrated Biomolecules: From Nucleic Acid Bases to DNA Segments. <i>Chemical Reviews</i> , 2012, 112, 5603-5640.	23.0	179
5525	4H-Dithieno[2,3-b:3'a'-e][1,4]thiazines – synthesis and electronic properties of a novel class of electron rich redox systems. <i>Chemical Communications</i> , 2012, 48, 7271.	2.2	21
5526	Fullerene C ₆₀ in Contact with Alkali Metal Clusters: Prototype Nano-Objects of Enhanced First Hyperpolarizabilities. <i>Journal of Physical Chemistry C</i> , 2012, 116, 11808-11819.	1.5	66
5527	Time-dependent density functional theory (TDDFT) modelling of Pechmann dyes: from accurate absorption maximum prediction to virtual dye screening. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 6682.	1.5	57
5528	Directions for Use of Density Functional Theory: A Short Instruction Manual for Chemists. , 2012, , 95-133.		2
5529	Weak Intermolecular Interactions: A Supermolecular Approach. , 2012, , 443-466.		9
5530	Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2012, , 573-610.		7
5531	Computational Mechanistic Study of Stereoselective Suzuki Coupling of an Î±-Cyano-Activated Secondary Alkyl. <i>Organometallics</i> , 2012, 31, 4610-4618.	1.1	13
5532	Joint electrical, photophysical and computational studies on D-Ï€-A dye sensitized solar cells: the impacts of dithiophene rigidification. <i>Chemical Science</i> , 2012, 3, 976.	3.7	140
5533	Theoretical study of Pd(0)-catalyzed carbohalogenation of alkenes: mechanism and origins of reactivities and selectivities in alkyl halide reductive elimination from Pd(ii) species. <i>Chemical Science</i> , 2012, 3, 1987.	3.7	90
5534	Probing the Electronic Structure of a Photoexcited Solar Cell Dye with Transient X-ray Absorption Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1695-1700.	2.1	63
5535	The entrance complex, transition state, and exit complex for the F + H ₂ O â†’ HF + OH reaction. Definitive predictions. Comparison with popular density functional methods. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10891.	1.3	63
5536	Accurate thermochemistry from a parameterized coupled-cluster singles and doubles model and a local pair natural orbital based implementation for applications to larger systems. <i>Journal of Chemical Physics</i> , 2012, 136, 064101.	1.2	68
5537	An Efficient and Accurate Formalism for the Treatment of Large Amplitude Intramolecular Motion. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2713-2724.	2.3	12
5538	Atomistic theory and simulation of the morphology and structure of ionic nanoparticles. <i>Nanoscale</i> , 2012, 4, 1051-1067.	2.8	15
5539	Single-crystal EPR and DFT study of a VAlâ€”Oâ€”VAl center in jeremejevite: electronic structure and 27Al hyperfine constants. <i>Physics and Chemistry of Minerals</i> , 2012, 39, 491-501.	0.3	5
5540	Thermochemical Properties and Bond Dissociation Energies of C ₃ -C ₅ Cycloalkyl Hydroperoxides and Peroxy Radicals: Cycloalkyl Radical + 3O ₂ Reaction Thermochemistry. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7550-7563.	1.1	13

#	ARTICLE	IF	CITATIONS
5541	Tunable Charge Tags for Electron-Based Methods of Peptide Sequencing: Design and Applications. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 608-620.	1.2	14
5542	Cascade Dissociations of Peptide Cation-Radicals. Part 2. Infrared Multiphoton Dissociation and Mechanistic Studies of $\langle b \rangle \langle i \rangle z \langle /i \rangle \langle /b \rangle$ -Ions from Pentapeptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 1351-1363.	1.2	28
5543	Telluroformaldehyde and its derivatives: structures, ionization potentials, electron affinities and singlet-triplet gaps of the X ₂ CTe and XYCTe (X, Y = ÅH, F, Cl, Br, I and CN) species. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	10
5544	Theoretical investigation of molecular excited states in polar organic monolayers via an efficient embedding approach. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	1
5545	Thermal and environmental effects on Oligothiophene low-energy singlet electronic excitations in dilute solution: a theoretical and experimental study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	7
5546	Impact of DFT functionals on the predicted magnesium-DNA interaction: an ONIOM study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	23
5547	Effects of mutations on the absorption spectra of copper proteins: a QM/MM study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	14
5548	Physicochemical characterization of environmental mutagens: 3-nitro-6-azabenz[a]pyrene and its N-oxide derivative. <i>Monatshefte für Chemie</i> , 2012, 143, 1123-1132.	0.9	7
5549	Theoretical study of BN ₄ : potential precursors of high energy density materials (HEDMs). <i>Journal of Molecular Modeling</i> , 2012, 18, 1927-1934.	0.8	5
5550	A QSAR study of radical scavenging antioxidant activity of a series of flavonoids using DFT based quantum chemical descriptors - the importance of group frontier electron density. <i>Journal of Molecular Modeling</i> , 2012, 18, 2621-2631.	0.8	69
5551	First- and second-row transition metal oxa-aza macrocyclic complexes: a DFT study of an octahedral conformation. <i>Journal of Molecular Modeling</i> , 2012, 18, 3243-3253.	0.8	8
5552	Can water be a catalyst on the HO ₂ +H ₂ O+O ₃ reactive cluster?. <i>Chemical Physics</i> , 2012, 399, 17-22.	0.9	19
5553	In situ FT-IR study of thiophene adsorbed on the surface of sulfided Mo catalysts. <i>Fuel</i> , 2012, 92, 77-83.	3.4	31
5554	Theoretical study of two states reactivity of methane activation on iron atom and iron dimer. <i>Fuel</i> , 2012, 96, 291-297.	3.4	24
5555	Bis(2-pyridylmethyl)alkyl(thioalkyl)diamines as promising scaffolds for the construction of fluorescent and redox chemosensors for transition and post-transition metal ions. <i>Inorganica Chimica Acta</i> , 2012, 381, 170-180.	1.2	7
5556	Thermodynamic and fluorescence emission properties of the Zn(II), Cd(II) and Pb(II) complexes with a fluorescent chelator bearing phenanthroline and naphthalene subunits. <i>Inorganica Chimica Acta</i> , 2012, 381, 229-235.	1.2	7
5557	Determination of zero-field splitting parameters for a MnIV center using variable-temperature, variable-field magnetic circular dichroism spectroscopy: Comparison to electron paramagnetic resonance spectroscopy. <i>Inorganica Chimica Acta</i> , 2012, 380, 135-140.	1.2	9
5558	Ground and excited state dynamics of new dinuclear ruthenium complexes: NMR, UV-Vis, IR, electrochemical, photophysical characterization, and theoretical study of Ru(bpy) ₂ (1/4-dpp)Ru(CN ⁻ X) _{4n+} complexes. <i>Inorganica Chimica Acta</i> , 2012, 387, 261-270.	1.2	1

#	ARTICLE	IF	CITATIONS
5559	Experimental, DFT and TD-DFT studies of rhenium complexes with thiocyanate ligands. <i>Inorganica Chimica Acta</i> , 2012, 387, 314-320.	1.2	17
5560	Twisted coordination mode of bis(N-heterocyclic carbene) ligands in octahedral geometry of group 6 transition metal complexes: Synthesis, structure, and reactivity. <i>Inorganica Chimica Acta</i> , 2012, 390, 199-209.	1.2	19
5561	New range-separated hybrids based on the TCA density functional. <i>Chemical Physics Letters</i> , 2012, 519-520, 145-149.	1.2	5
5562	Assessment of chemical core potentials for the computation on enthalpies of formation of transition-metal complexes. <i>Chemical Physics Letters</i> , 2012, 521, 150-156.	1.2	12
5563	Theoretical study of intermolecular magnetic interaction of chromium(V) nitrido complex self-assembly with tetradentate Schiff base ligand. <i>Chemical Physics Letters</i> , 2012, 523, 65-68.	1.2	2
5564	Topological (ELF and $\tilde{\chi}$) study of the unusually long N=O bond in (CF ₃) ₂ NO=NO. <i>Chemical Physics Letters</i> , 2012, 525-526, 24-31.	1.2	6
5565	Performance improvement of dye-sensitizing solar cell by semi-rigid triarylamine-based donors. <i>Dyes and Pigments</i> , 2012, 94, 40-48.	2.0	41
5566	Protonation sites in peptide dications and cation-radicals containing β^2 -amino acid residues. <i>International Journal of Mass Spectrometry</i> , 2012, 316-318, 57-67.	0.7	5
5567	Elimination of water from the backbone of protonated tetraglycine. <i>International Journal of Mass Spectrometry</i> , 2012, 316-318, 268-272.	0.7	11
5568	Fragmentations of protonated cyclic-glycylglycine and cyclic-alanylalanine. <i>International Journal of Mass Spectrometry</i> , 2012, 316-318, 199-205.	0.7	14
5569	Synthesis, characterization and evaluation of computationally designed nanoparticles of molecular imprinted polymers as drug delivery systems. <i>International Journal of Pharmaceutics</i> , 2012, 424, 67-75.	2.6	65
5570	DFT and surface-enhanced Raman scattering study of tryptophan silver complex. <i>Journal of Colloid and Interface Science</i> , 2012, 380, 141-149.	5.0	68
5571	An innovative method for the non-destructive identification of photodegradation products in solid state: ¹ H= ¹⁴ N NMR= NQR and DFT/QTAIM study of photodegradation of nifedipine (anti-hypertensive) to nitrosonifedipine (potential anti-oxidative). <i>European Journal of Pharmaceutical Sciences</i> , 2012, 47, 97-107.	1.9	11
5572	Density functional calculations on the effect of sulfur substitution for 2-hydroxypropyl-p-nitrophenyl phosphate: C O vs. P O bond cleavage. <i>Bioorganic Chemistry</i> , 2012, 40, 99-107.	2.0	2
5573	N-(4-Substituted-benzoyl)-N-(β -D-glucopyranosyl)ureas as inhibitors of glycogen phosphorylase: Synthesis and evaluation by kinetic, crystallographic, and molecular modelling methods. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 1801-1816.	1.4	13
5574	Theoretical Studies of QSAR and Molecular Design on a Novel Series of Ethynyl=Quinolinecarbonitriles as Src Inhibitors. <i>Chemical Biology and Drug Design</i> , 2012, 80, 134-147.	1.5	8
5575	Ligand=and Structure=Based Drug Design Strategies and PPAR α/β Selectivity. <i>Chemical Biology and Drug Design</i> , 2012, 80, 533-544.	1.5	8
5576	IR and Raman spectra of nitroanthracene isomers: Substitutional effects based on density functional theory study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 89, 129-136.	2.0	12

#	ARTICLE	IF	CITATIONS
5577	â€œAdditiveâ€ cooperativity of hydrogen bonds in complexes of catechol with proton acceptors in the gas phase: FTIR spectroscopy and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 75-82.	2.0	7
5578	Theoretical and experimental study on the excited states of the X-, $\hat{1}\pm$ - and $\hat{1}^2$ -forms of lithium phthalocyanine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 118-125.	2.0	9
5579	Quantum mechanical study and spectroscopic (FT-IR, FT-Raman, ^{13}C , ^1H , UV) study, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 4-[(4-aminobenzene) sulfonyl] aniline by ab initio HF and density functional method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 92, 154-163.	2.0	136
5580	Vibrational spectroscopic investigation on the structure of 2-ethylpyridine-4-carbothioamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 93, 214-222.	2.0	55
5581	Molecular structure refinement by direct fitting of atomic coordinates to experimental ESR spectra. <i>Journal of Magnetic Resonance</i> , 2012, 216, 62-68.	1.2	4
5582	Photoprotective capacities of lichen metabolites: A joint theoretical and experimental study. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2012, 111, 17-26.	1.7	31
5583	A computational comparison of NiII and PtII hydrido-tris(pyrazolyl)borate supported hydroarylation catalysis. <i>Journal of Molecular Catalysis A</i> , 2012, 353-354, 1-6.	4.8	2
5584	The effect of side chain connectivity and local hydration on proton transfer in 3M perfluorosulfonic acid membranes. <i>Solid State Ionics</i> , 2012, 213, 83-91.	1.3	31
5585	Toward n-channel organic thin film transistors based on a distyryl-bithiophene derivatives. <i>Tetrahedron</i> , 2012, 68, 4664-4671.	1.0	5
5586	Syntheses and conformational analyses of new naphth[1,2-e][1,3]oxazino[3,2-c]quinazolin-13-ones. <i>Tetrahedron</i> , 2012, 68, 4600-4608.	1.0	12
5587	The first synthesis of spirocyclopentyl derivatives of lupane triterpenoids by radical nitrocyclization of C-2-diallyl substituted betulonates. <i>Tetrahedron Letters</i> , 2012, 53, 217-221.	0.7	5
5588	Efficient sonochemical synthesis of alkyl 4-aryl-6-chloro-5-formyl-2-methyl-1,4-dihydropyridine-3-carboxylate derivatives. <i>Ultrasonics Sonochemistry</i> , 2012, 19, 221-226.	3.8	17
5589	On the accuracy of the non-self-consistent calculation of the electronic structure of solids with hybrid functionals. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012, 376, 879-882.	0.9	23
5590	New oxidovanadium(V) complexes of the cation $[\text{VO}]^{3+}$: Synthesis, structural characterization and DFT studies. <i>Polyhedron</i> , 2012, 36, 21-29.	1.0	13
5591	Synthesis, structural and optical studies of several new ditelluroether iodides. <i>Polyhedron</i> , 2012, 39, 106-112.	1.0	4
5592	Theoretical investigation of astacin proteolysis. <i>Journal of Inorganic Biochemistry</i> , 2012, 111, 70-79.	1.5	17
5593	Binding of TNT to amplifying fluorescent polymers: An ab initio and molecular dynamics study. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 33, 12-18.	1.3	12
5594	Theoretical study on the electronic structure and optical properties of carbazole- iC -dimesitylborane as bipolar fluorophores for nondoped blue OLEDs. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 34, 46-56.	1.3	16

#	ARTICLE	IF	CITATIONS
5595	Geometric parameters and energies of molecular structures of macrocyclic metal chelates in the ternary 3d M(II) ion-ethanedithioamide-ethanedial systems according to quantum-chemical DFT B3LYP calculations. Russian Journal of Inorganic Chemistry, 2012, 57, 205-210.	0.3	27
5596	Theoretical survey of the reaction between osmium and acetaldehyde. Russian Journal of Physical Chemistry A, 2012, 86, 798-804.	0.1	2
5597	Incorporation of Manganese Complexes into Xylanase: New Artificial Metalloenzymes for Enantioselective Epoxidation. ChemBioChem, 2012, 13, 240-251.	1.3	72
5598	Electrolysis of Water in the Diffusion Layer: First-Principles Molecular Dynamics Simulation. Chemistry - A European Journal, 2012, 18, 277-282.	1.7	13
5599	Do Glycosyl Sulfonium Ions Engage in Neighbouring-Group Participation? A Study of Oxathiane Glycosyl Donors and the Basis for their Stereoselectivity. Chemistry - A European Journal, 2012, 18, 321-333.	1.7	45
5600	Mechanistic Studies on a Sulfoxide Transfer Reaction Mediated by Diphenyl Sulfoxide/Triflic Anhydride. Chemistry - A European Journal, 2012, 18, 2987-2997.	1.7	28
5601	Reactions of Vinylidenecyclopropanes with Diphenyl Diselenide in the Presence of AIBN and Thermally-Induced Further Transformations. Chemistry - A European Journal, 2012, 18, 1280-1285.	1.7	11
5602	Hydrogen abstraction reactions of OH radicals with $\text{CH}_3\text{CH}_2\text{CH}_2\text{Cl}$ and $\text{CH}_3\text{CHClCH}_3$: A mechanistic and kinetic study. Journal of Computational Chemistry, 2012, 33, 66-75.	1.5	7
5603	Empirical formulation and parameterization of cation- π interactions for protein modeling. Journal of Computational Chemistry, 2012, 33, 153-162.	1.5	17
5604	Multifn: A multifunctional wavefunction analyzer. Journal of Computational Chemistry, 2012, 33, 580-592.	1.5	21,818
5605	Radical Chemistry of Iminepyridine Ligands. European Journal of Inorganic Chemistry, 2012, 2012, 530-534.	1.0	38
5606	Snapshots of a Reversible Metal-Ligand Two-Electron Transfer Step Involving Compounds Related by Multiple Types of Isomerism. European Journal of Inorganic Chemistry, 2012, 2012, 512-519.	1.0	15
5607	Cu-Catalyzed Enantioselective 1,4-Additions of Aryl Grignard Reagents to Cyclohexenone in the Presence of TADDOL-Derived Phosphane-Phosphite Ligands. European Journal of Organic Chemistry, 2012, 2012, 1179-1185.	1.2	23
5608	Chemical activation reactions of cyclic alkanes and ethers and tricyclodecane ring-opened diradicals with O_2 : Thermochemistry, reaction paths, kinetics, and modeling. International Journal of Chemical Kinetics, 2012, 44, 232-256.	1.0	4
5609	Gas-phase doubly charged complexes of cyclic peptides with copper in +1, +2 and +3 formal oxidation states: formation, structures and electron capture dissociation. Journal of Mass Spectrometry, 2012, 47, 208-220.	0.7	17
5610	Activation of Ziegler-Natta catalysts by organohalide promoters: A combined experimental and density functional theory study. Journal of Applied Polymer Science, 2012, 123, 2526-2533.	1.3	26
5611	Highly Efficient Aerobic Oxidative Hydroxylation of Arylboronic Acids: Photoredox Catalysis Using Visible Light. Angewandte Chemie - International Edition, 2012, 51, 784-788.	7.2	442
5612	The Early Life of a Peptide Cation-Radical. Ground and Excited-State Trajectories of Electron-Based Peptide Dissociations During the First 330 Femtoseconds. Journal of the American Society for Mass Spectrometry, 2012, 23, 446-459.	1.2	25

#	ARTICLE	IF	CITATIONS
5613	Ab initio classical trajectory calculations of 1,3-cyclobutanedione radical cation dissociation. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	4
5614	Spin-Selective Electron Transfer and Charge Recombination in Self-Assembled Porphyrin Naphthalenediimide Dyads. <i>Applied Magnetic Resonance</i> , 2012, 42, 41-55.	0.6	7
5615	A comparative study of the hydrogen-bonding patterns and prototropism in solid 2-thiocytosine (potential antileukemic agent) and cytosine, as studied by 1H-14N NQDR and QTAIM/ DFT. <i>Journal of Molecular Modeling</i> , 2012, 18, 11-26.	0.8	12
5616	Molecular electrostatic potentials of DNA base-base pairing and mispairing. <i>Journal of Molecular Modeling</i> , 2012, 18, 91-101.	0.8	23
5617	Noscapinoids with anti-cancer activity against human acute lymphoblastic leukemia cells (CEM): a three dimensional chemical space pharmacophore modeling and electronic feature analysis. <i>Journal of Molecular Modeling</i> , 2012, 18, 307-318.	0.8	17
5618	Selective complexation of alkali metal ions using crown ethers derived from calix[4]arenes: a computational investigation of the structural and energetic factors. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2013, 75, 185-195.	1.6	2
5619	Perturbing Peptide Cation-Radical Electronic States by Thioxoamide Groups: Formation, Dissociations, and Energetics of Thioxopeptide Cation-Radicals. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1265-1275.	1.1	7
5620	Aromatic Interactions as Control Elements in Stereoselective Organic Reactions. <i>Accounts of Chemical Research</i> , 2013, 46, 979-989.	7.6	216
5621	A theoretical study on the hydrogen transport mechanism in SrTiO ₃ perovskite. II. Scandium doping at titanium site. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 599-604.	1.0	5
5622	Polarized-unpolarized ground state of small polycyclic aromatic hydrocarbons. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 815-819.	1.0	8
5623	Inverse sandwich complexes based on low-valent group 13 elements and cyclobutadiene: A theoretical investigation on E ₄ H ₄ (E = Al, Ga, In, Tl). <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1018-1025.	1.0	7
5624	Quantum chemical investigation on the reaction mechanism of tertiary phosphines with unsaturated carboxylic acids: An insight into kinetic data. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1086-1094.	1.0	17
5625	TDDFT Investigation of the Electronic Structures and Photophysical Properties of Fluorescent Extended Styryl Push-Pull Chromophores Containing Carbazole Unit. <i>Journal of Fluorescence</i> , 2013, 23, 1121-1138.	1.3	22
5626	Synthesis, Photo-physical and DFT Studies of ESIPT Inspired Novel 2-(2,4-Dihydroxyphenyl) Benzimidazole, Benzoxazole and Benzothiazole. <i>Journal of Fluorescence</i> , 2013, 23, 1019-1029.	1.3	44
5627	A Combined Experimental and DFT-TDDFT Study of the Excited-State Intramolecular Proton Transfer (ESIPT) of 2-(2-Hydroxyphenyl) Imidazole Derivatives. <i>Journal of Fluorescence</i> , 2013, 23, 839-851.	1.3	32
5628	Electron Transfer Dissociation of Photolabeled Peptides. Backbone Cleavages Compete with Diazirine Ring Rearrangements. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 1641-1653.	1.2	19
5629	Does Addition of NO ₂ to Carbon-Centered Radicals Yield RONO or RNO ₂ ? An Investigation Using Distonic Radical Ions. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 481-492.	1.2	5
5630	Fragmentation Chemistry of [Met-Gly] ⁺ , [Gly-Met] ⁺ , and [Met-Met] ⁺ Radical Cations. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 543-553.	1.2	4

#	ARTICLE	IF	CITATIONS
5649	Structural, Spectroscopic, and Computational Characterization of the Azide Adduct of Fe ^{III} (2,6-diacetylpyridinebis(semioxamazide)), a Functional Analogue of Iron Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2013, 52, 8909-8918.	1.9	9
5650	Linear-scaling self-consistent field methods for large molecules. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 614-636.	6.2	88
5651	Mercury(II) complexes with 5-methyl-5-(4-pyridyl)-2,4-imidazolidenedione: Synthesis, structural characterization, and theoretical studies. <i>Journal of Molecular Structure</i> , 2013, 1051, 15-22.	1.8	11
5652	Nuclear wastefrom materials: Atomistic simulation case studies. <i>Journal of Nuclear Materials</i> , 2013, 441, 29-39.	1.3	45
5653	A DFT study of the vicinal 3J(119Sn,13C) and 3J(119Sn,1H) coupling constants in trimethyl- and chlorodimethylstannyl propanoates. <i>Journal of Organometallic Chemistry</i> , 2013, 724, 139-146.	0.8	8
5654	Conformational analysis of some N,N-diethyl-2-[(4-substituted) phenylthio] acetamides. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 738-746.	2.0	9
5655	Dancing multiplicity states supported by a carboxylated group in dicopper structures bonded to O ₂ . <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	12
5656	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in <i>p</i> -nitroaniline. <i>Molecular Physics</i> , 2013, 111, 1235-1248.	0.8	79
5657	Restricted Rotation of C-F Bonds through a Rigidified Donor Structure to Increase the ICT Ability of Platinum-Acetylide-Based DSSCs. <i>Chemistry - an Asian Journal</i> , 2013, 8, 2660-2669.	1.7	14
5658	Hybrid density functional based study on the band structure of trioctahedral mica and its dependence on the variation of Fe ²⁺ content. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 44, 129-135.	1.3	5
5659	Anchor position and donor/acceptor effects on transport properties in fused benzene-substituted oligothiophene molecular device. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2013, 54, 247-252.	1.3	2
5660	Surface species formed during thermal transformation of ethanol on ZnO powder. <i>Journal of Catalysis</i> , 2013, 300, 163-173.	3.1	28
5661	Novel blue luminescent materials for organic light-emitting diodes based on C ₉ -fluorenyl anthracenes. <i>Dyes and Pigments</i> , 2013, 96, 642-652.	2.0	22
5662	Chiroptical Properties of Carbo[6]Helicene Derivatives Bearing Extended Conjugated Cyano Substituents. <i>Chirality</i> , 2013, 25, 455-465.	1.3	36
5663	Performance of conventional and dispersion-corrected density-functional theory methods for hydrogen bonding interaction energies. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 12821.	1.3	120
5664	Study of the Gas-Phase Oxygen-Hydrogen Exchange Reaction of O(³ P) + <i>i</i> -C ₃ H ₇ + H(² S) + CH ₃ COCH ₃ . <i>Journal of Physical Chemistry A</i> , 2013, 117, 12020-12025.	1.1	4
5665	Systematic development of predictive molecular models of high surface area activated carbons for adsorption applications. <i>Carbon</i> , 2013, 64, 262-280.	5.4	76
5666	Pyridinium-based tripodal chemosensor in visual sensing of AMP in water by indicator displacement assay (IDA). <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 5666.	1.5	19

#	ARTICLE	IF	CITATIONS
5667	Molecular and Electronic Structure Basis of the Ambipolar Behavior of Naphthalimide-Terthiophene Derivatives: Implementation in Organic Field-Effect Transistors. <i>Chemistry - A European Journal</i> , 2013, 19, 12458-12467.	1.7	37
5668	Theoretical study on the electronic structure, formation and absorption spectra of lithium, sodium and potassium complexes of N-confused tetraphenylporphyrin. <i>Computational and Theoretical Chemistry</i> , 2013, 1020, 38-50.	1.1	7
5669	Geometric and Electronic Structures of Manganese-Substituted Iron Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2013, 52, 3356-3367.	1.9	19
5670	Reactivity and catalysis by nanoalloys. , 2013, , 283-344.		1
5671	Chemo- and diastereoselective tandem dual oxidation of B(pin)-substituted allylic alcohols: synthesis of B(pin)-substituted epoxy alcohols, 2-keto-anti-1,3-diols and dihydroxy-tetrahydrofuran-3-ones. <i>Chemical Science</i> , 2013, 4, 3946.	3.7	11
5672	Aromatic interactions in asymmetric catalysis: control of enantioselectivity in Diels-Alder reactions catalysed by camphor-derived hydrazides. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 5226.	1.5	10
5673	Computational Analysis of ^{47/49} Ti NMR Shifts and Electric Field Gradient Tensors of Half-Titanocene Complexes: Structure-Bonding-Property Relationships. <i>Chemistry - A European Journal</i> , 2013, 19, 12018-12033.	1.7	12
5674	Theoretical investigation of the donor group related electronic structure properties in push-pull organic sensitizers. <i>RSC Advances</i> , 2013, 3, 6030.	1.7	22
5675	Substituted group and side chain effects for the porphyrin and zinc(II)-porphyrin derivatives: A DFT and TD-DFT study. <i>Journal of Luminescence</i> , 2013, 142, 8-16.	1.5	21
5676	Polymorphic Co-crystals from Polymorphic Co-crystal Formers: Competition between Carboxylic Acid-Pyridine and Phenol-Pyridine Hydrogen Bonds. <i>Crystal Growth and Design</i> , 2013, 13, 3935-3952.	1.4	80
5677	QM/MM description of platinum-DNA interactions: comparison of binding and DNA distortion of five drugs. <i>RSC Advances</i> , 2013, 3, 4066.	1.7	30
5678	Anion and ion-pair binding by a G-2 poly(ethylene imine) dendrimer. <i>Dalton Transactions</i> , 2013, 42, 12130.	1.6	6
5679	The effect of hydrogen passivation on Si nanocrystals: Surface and spin states. <i>Computational and Theoretical Chemistry</i> , 2013, 1019, 125-131.	1.1	4
5680	Electrocatalysis in Fuel Cells. <i>Lecture Notes in Energy</i> , 2013, , .	0.2	85
5681	A conformational study of hydroxylated isoflavones by vibrational spectroscopy coupled with DFT calculations. <i>Vibrational Spectroscopy</i> , 2013, 68, 257-265.	1.2	16
5682	QSAR modeling of aromatase inhibitory activity of 1-substituted 1,2,3-triazole analogs of letrozole. <i>European Journal of Medicinal Chemistry</i> , 2013, 69, 99-114.	2.6	31
5683	Aryl pyrazaboles: a new class of tunable and highly fluorescent materials. <i>Dalton Transactions</i> , 2013, 42, 16614.	1.6	19
5684	Structural and elastic properties of Ce2O3 under pressure from LDA+U method. <i>Frontiers of Physics</i> , 2013, 8, 405-411.	2.4	6

#	ARTICLE	IF	CITATIONS
5685	Molecular Engineering of Indoline-Based Dâ€“Aa~i€“A Organic Sensitizers toward High Efficiency Performance from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17382-17398.	1.5	79
5686	Stereoselective synthesis of highly functionalized tetrahydrocarbazoles through a domino Michaelâ€“Henry reaction: an easy access to four contiguous chiral centers. <i>RSC Advances</i> , 2013, 3, 10644.	1.7	26
5687	Theoretical studies of structure, energetics and properties of Ca ²⁺ complexes with alizarin glucoside. <i>Journal of Molecular Modeling</i> , 2013, 19, 4209-4214.	0.8	5
5688	Analysis of the Gas Phase Reactivity of Chlorosilanes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5221-5231.	1.1	47
5689	Specifics of molecular structures of (565)macrotricyclic 3d-Metal chelates in the ternary systems M(II)-hydrazinecarbothioamide-2,4-Pentanedione according to DFT calculations. <i>Russian Journal of Inorganic Chemistry</i> , 2013, 58, 548-553.	0.3	11
5690	Molecular structure and thermodynamic parameters of (5656)macrotetracyclic chelates in the 3d-element(ii) ion-hydrazinomethanethiohydrazide-2,3-butanedione ternary system according to density functional quantum-chemical calculations. <i>Russian Journal of Inorganic Chemistry</i> , 2013, 58, 174-179.	0.3	27
5691	Experimental and theoretical studies for mild steel corrosion inhibition in 1M HCl by two new benzothiazine derivatives. <i>Corrosion Science</i> , 2013, 76, 317-324.	3.0	131
5692	Comparative stability of isomeric (565)macrotricyclic chelates of 3d-elements formed in the systems M(II)-thiosemicarbazide-formaldehyde according to DFT B3LYP data. <i>Russian Journal of General Chemistry</i> , 2013, 83, 1123-1130.	0.3	4
5693	Calix[4]resorcinols bearing $\hat{1}^3$ -aminoacetal groups on the upper rim. Synthesis and properties. <i>Russian Journal of General Chemistry</i> , 2013, 83, 319-324.	0.3	3
5694	Density functional theory study of Te(CN) ₂ , Te(CN)(NC), and Te(NC) ₂ and their isomerizations. <i>Structural Chemistry</i> , 2013, 24, 2047-2057.	1.0	7
5695	Theoretical study on the kinetics and branching ratios of the gas phase reactions of 1, 1-Dichlorodimethylether (DCDME) with Cl atom. <i>Structural Chemistry</i> , 2013, 24, 1621-1626.	1.0	11
5696	Computational mechanistic study of methanol and molecular oxygen reaction on the triplet and singlet potential energy surfaces. <i>Structural Chemistry</i> , 2013, 24, 1051-1062.	1.0	5
5697	Avoiding pitfalls of a theoretical approach: the harmonic oscillator measure of aromaticity index from quantum chemistry calculations. <i>Structural Chemistry</i> , 2013, 24, 1171-1184.	1.0	31
5698	A computational investigation on the potential energy surface of thiosulfeno with O(3P) reaction. <i>Structural Chemistry</i> , 2013, 24, 517-522.	1.0	4
5699	First-principles investigations on polytypes of BaTiO ₃ : Hybrid calculations and pressure dependences. <i>Journal of the Korean Physical Society</i> , 2013, 62, 1629-1635.	0.3	7
5700	The interaction between carbon nanotube and skin anti-cancer drugs: a DFT and NBO approach. <i>Journal of Nanostructure in Chemistry</i> , 2013, 3, 1.	5.3	27
5701	Comparative amino acid decomposition analysis of potent type I p38 $\hat{1}$ ± inhibitors. <i>DARU, Journal of Pharmaceutical Sciences</i> , 2013, 21, 41.	0.9	4
5702	Synthesis and Ligand Non-Innocence of Thiolate-Ligated (N4S) Iron(II) and Nickel(II) Bis(imino)pyridine Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 10467-10480.	1.9	21

#	ARTICLE	IF	CITATIONS
5703	Efficient in Situ Synthesis of 3,5-Disubstituted-1,2,4-triazoles Under Microwave-Assisted Conditions. <i>Synthetic Communications</i> , 2013, 43, 3181-3191.	1.1	9
5704	Structure of genipin in solution: a combined experimental and theoretical study. <i>RSC Advances</i> , 2013, 3, 13764.	1.7	15
5705	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. , 2013, , 1-57.		1
5706	Electron Density Analysis. , 2013, , 187-226.		21
5707	NMR Spectroscopy in Inorganic Chemistry. , 2013, , 381-406.		0
5708	Synthesis, structure, and transformations of N-(bicyclo[2.2.1]hept-5-en-endo-2-ylmethyl)-N-[(oxiran-2-yl) methyl]-arenesulfonamides. <i>Russian Journal of Organic Chemistry</i> , 2013, 49, 1122-1134.	0.3	1
5709	Reaction Pathways and Energetics of Etheric C=O Bond Cleavage Catalyzed by Lanthanide Triflates. <i>ACS Catalysis</i> , 2013, 3, 1908-1914.	5.5	48
5710	δ^2 -Oxygen Effect in the Barton-McCombie Deoxygenation Reaction: Further Experimental and Theoretical Findings. <i>Journal of Organic Chemistry</i> , 2013, 78, 9127-9136.	1.7	8
5711	Computational modeling of the direct hydride transfer mechanism for the MAO catalyzed oxidation of phenethylamine and benzylamine: ONIOM (QM/QM) calculations. <i>Journal of Neural Transmission</i> , 2013, 120, 937-945.	1.4	55
5712	Theoretical studies on the reaction mechanism of PP1 and the effects of different oxidation states of the Mn-Mn center on the mechanism. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 451-459.	1.1	11
5713	Gaining insight into the chemistry of lipoxygenases: a computational investigation into the catalytic mechanism of (8R)-lipoxygenase. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 343-355.	1.1	11
5714	Electron correlation effects and density analysis of the first-order hyperpolarizability of neutral guanine tautomers. <i>Journal of Molecular Modeling</i> , 2013, 19, 3095-3102.	0.8	8
5715	Density functional studies on photophysical properties and chemical reactivities of the triarylboranes: effect of the constraint of planarity. <i>Journal of Molecular Modeling</i> , 2013, 19, 3437-3446.	0.8	11
5716	Half-metallicity of graphene nanoribbons and related systems: a new quantum mechanical El Dorado for nanotechnologies or a hype for materials scientists?. <i>Journal of Molecular Modeling</i> , 2013, 19, 2699-2714.	0.8	10
5717	Explaining reaction mechanisms using the dual descriptor: a complementary tool to the molecular electrostatic potential. <i>Journal of Molecular Modeling</i> , 2013, 19, 2715-2722.	0.8	44
5718	An intermediate level of approximation for computing the dual descriptor. <i>Journal of Molecular Modeling</i> , 2013, 19, 2811-2820.	0.8	2
5719	Electronic structures of bisnoradamantanyl and bisnoradamantanyl dications and related species. <i>Journal of Molecular Modeling</i> , 2013, 19, 2485-2497.	0.8	4
5720	Role of gold in a complex cascade reaction involving two electrocyclization steps. <i>Journal of Molecular Modeling</i> , 2013, 19, 1981-1984.	0.8	1

#	ARTICLE	IF	CITATIONS
5721	Cyano or o-nitrophenyl? Which is the optimal electron-withdrawing group for the acrylic acid acceptor of D- π -A sensitizers in DSSCs? A density functional evaluation. <i>Journal of Molecular Modeling</i> , 2013, 19, 1597-1604.	0.8	29
5722	Through-bond instability in polyphenol tautomers. <i>Tetrahedron Letters</i> , 2013, 54, 1452-1455.	0.7	6
5723	Hidden Non-Innocence in an Expanded Porphyrin: Electronic Structure of the Siamese-Twin Porphyrin's Dicopper Complex in Different Oxidation States. <i>Journal of the American Chemical Society</i> , 2013, 135, 13892-13899.	6.6	48
5724	The failure of UMP2 on the keto \rightleftharpoons enol tautomerization of $\dot{\text{I}}^2$ -radical compounds: The effect of spin contamination. <i>Chemical Physics Letters</i> , 2013, 565, 18-21.	1.2	3
5725	Electrostatic Potential of Insulin: Exploring the Limitations of Density Functional Theory and Force Field Methods. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3978-3985.	2.3	42
5726	Molecular Catch Bonds and the Anti-Hammond Effect in Polymer Mechanochemistry. <i>Journal of the American Chemical Society</i> , 2013, 135, 12722-12729.	6.6	118
5727	Efficient self-consistent treatment of electron correlation within the random phase approximation. <i>Journal of Chemical Physics</i> , 2013, 139, 084113.	1.2	81
5728	Synthesis and Structure-Activity Relationship (SAR) of 2-Methyl-4-oxo-3-oxetanylcabamic Acid Esters, a Class of Potent <i>N</i> -Acylethanolamine Acid Amidase (NAAA) Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 6917-6934.	2.9	43
5729	Gambogic Acid Is a Tissue-Specific Proteasome Inhibitor <i>In Vitro</i> and <i>In Vivo</i> . <i>Cell Reports</i> , 2013, 3, 211-222.	2.9	93
5730	Copper interacts with nonylphenol to cancel the effect of nonylphenol on fish chemosensory behaviour. <i>Aquatic Toxicology</i> , 2013, 142-143, 203-209.	1.9	8
5731	Analysis of matrine-type alkaloids using ESI-QTOF. <i>International Journal of Mass Spectrometry</i> , 2013, 341-342, 28-33.	0.7	13
5732	Synthesis and characterization of dianchoring organic dyes containing 2,7-diaminofluorene donors as efficient sensitizers for dye-sensitized solar cells. <i>Organic Electronics</i> , 2013, 14, 3267-3276.	1.4	22
5733	The role of (5 ϵ -R) and (5 ϵ -S) 5 ϵ ,8-cyclo-2 ϵ -deoxyadenosine in ds-DNA structure. <i>Computational and Theoretical Chemistry</i> , 2013, 1010, 38-44.	1.1	8
5734	Applying vibrational spectroscopy to the study of nucleobases \rightleftharpoons adenine as a case-study. <i>New Journal of Chemistry</i> , 2013, 37, 2691.	1.4	36
5735	Revealing the nature of intermolecular interaction and configurational preference of the nonpolar molecular dimers (H ₂) ₂ , (N ₂) ₂ , and (H ₂)(N ₂). <i>Journal of Molecular Modeling</i> , 2013, 19, 5387-5395.	0.8	129
5736	On the Nature of Interactions of Radicals with Polar Molecules. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12560-12568.	1.1	12
5737	Theoretical studies on the reductive elimination reaction mechanism from neutral palladium(IV) sulfinate complexes. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 933-938.	0.9	8
5738	Many-body Green's function <i>GW</i> and Bethe-Salpeter study of the optical excitations in a paradigmatic model dipeptide. <i>Journal of Chemical Physics</i> , 2013, 139, 194308.	1.2	52

#	ARTICLE	IF	CITATIONS
5740	DFT investigation of the intermolecular interactions of a thieno-separated tricyclic guanine analog with gold nanoclusters. <i>Computational and Theoretical Chemistry</i> , 2013, 1019, 1-10.	1.1	6
5741	Gas-phase structures of phosphopeptide ions: A difficult case. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 249-256.	0.7	24
5742	Effect of Zn ²⁺ and temperature on the conformational equilibrium of single-stranded polyA in neutral solutions. <i>International Journal of Biological Macromolecules</i> , 2013, 61, 448-452.	3.6	4
5743	Investigation on the adsorption characteristics of anserine on the surface of colloidal silver nanoparticles. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 112, 27-32.	2.0	26
5744	Structural and Charge Sensitivity of Surface-Enhanced Raman Spectroscopy of Adenine on Silver Surface: A Quantum Chemical Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23730-23737.	1.5	40
5745	Computational Modeling of Octahedral Iron Oxide Clusters: Hexaaquairon(III) and Its Dimers. <i>Journal of Physical Chemistry C</i> , 2013, 117, 21706-21717.	1.5	19
5746	High-power Broadband Organic THz Generator. <i>Scientific Reports</i> , 2013, 3, 3200.	1.6	125
5747	Nicotinamide Phosphoribosyltransferase Inhibitors, Design, Preparation, and Structure-Activity Relationship. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 9071-9088.	2.9	32
5748	The OH-initiated atmospheric oxidation of cyclopentene: A coupled-cluster study of the potential energy surface. <i>Chemical Physics Letters</i> , 2013, 579, 35-39.	1.2	7
5749	Combined experimental and DFT/TDDFT study of photo-active constituents of <i>Canarium odontophyllum</i> for DSSC application. <i>Chemical Physics Letters</i> , 2013, 585, 121-127.	1.2	46
5750	Electronic structure analysis of isomeric preferences of canonical and zwitterionic forms of lornoxicam. <i>Computational and Theoretical Chemistry</i> , 2013, 1023, 51-58.	1.1	4
5751	Heterometallic Aluminum-Chromium Phenazine and Thiophenazine Complexes. Formation of a Tetranuclear Chromium(I) Sandwich Complex. <i>Organometallics</i> , 2013, 32, 2329-2335.	1.1	11
5752	Evaluating push-pull dye efficiency using TD-DFT and charge transfer indices. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20210.	1.3	68
5753	Role of the plasmon-pole model in the G W approximation. <i>Physical Review B</i> , 2013, 88, .		65
5754	Nitro aci-nitro tautomerism and E/Z isomeric preferences of nitroethenediamine derivatives: a quantum chemical study. <i>RSC Advances</i> , 2013, 3, 25268.	1.7	12
5755	Synthesis and Properties of Thiophene and Dithiin Functionalized Tetrathiafulvalenes. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2013, 188, 1835-1844.	0.8	3
5756	Density functional molecular dynamics simulations investigation of proton transfer and inter-molecular reorientation under external electrostatic field perturbation: Case studies for water and imidazole systems. <i>Journal of Power Sources</i> , 2013, 229, 141-148.	4.0	4
5757	Application of Time-Dependent Density Functional Theory and Optical Spectroscopy toward the Rational Design of Novel 3,4,5-Triaryl-1-R-1,2-diphospholes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6827-6834.	1.1	24

#	ARTICLE	IF	CITATIONS
5758	A highly reactive ($\leq 1\text{ min}$) ratiometric chemodosimeter for selective "naked eye" and fluorogenic detection of hydrazine. RSC Advances, 2013, 3, 18872.	1.7	57
5759	A Density Functional Theory Investigation into the Binding of the Antioxidants Ergothioneine and Ovothiol to Copper.. Journal of Physical Chemistry A, 2013, 117, 4057-4065.	1.1	23
5760	Theoretical prediction of rare gas inserted hydronium ions: HRgOH ₂ ⁺ . Journal of Chemical Physics, 2013, 138, 194308.	1.2	21
5761	Isolated catalyst sites on amorphous supports: A systematic algorithm for understanding heterogeneities in structure and reactivity. Journal of Chemical Physics, 2013, 138, 204105.	1.2	41
5762	Thio Effects and an Unconventional Metal Ion Rescue in the Genomic Hepatitis Delta Virus Ribozyme. Biochemistry, 2013, 52, 6499-6514.	1.2	50
5763	Substituent Effect on the Photoreduction Kinetics of Benzophenone. Journal of Physical Chemistry A, 2013, 117, 10196-10210.	1.1	26
5764	Bandgap bowing in Ta-W-O system for efficient solar energy conversion: Insights from density functional theory and X-ray diffraction. Applied Physics Letters, 2013, 103, 133905.	1.5	9
5765	Real-Space Density Functional Theory on Graphical Processing Units: Computational Approach and Comparison to Gaussian Basis Set Methods. Journal of Chemical Theory and Computation, 2013, 9, 4360-4373.	2.3	53
5766	Enhancing the Thermoelectric Properties of Layered Transition-Metal Dichalcogenides 2H-MQ ₂ (M = Mo, W; Q = S, Se, Te) by Layer Mixing: Density Functional Investigation. Chemistry of Materials, 2013, 25, 3745-3752.	3.2	81
5767	Spectral Signatures of Perylene Diimide Derivatives: Insights From Theory. Journal of Physical Chemistry C, 2013, 117, 21682-21691.	1.5	13
5768	Construction of six-membered nitrogen-heterocycles via intramolecular cyclization of iminyl radical: A theoretical perspective. Computational and Theoretical Chemistry, 2013, 1025, 52-57.	1.1	3
5769	Features in the electronic structure and photoemission spectra of organic molecular semiconductors: The molecules of metal-phthalocyanines and PTCDA. JETP Letters, 2013, 98, 14-18.	0.4	2
5770	Dynamical Treatment of Charge Transfer through Duplex Nucleic Acids Containing Modified Adenines. ACS Nano, 2013, 7, 9396-9406.	7.3	8
5771	Toward a Realistic Modeling of the Photophysics of Molecular Building Blocks for Energy Harvesting: The Charge-Transfer State in 4,7-Dithien-2-yl-2,1,3-benzothiadiazole As a Case Study. Journal of Physical Chemistry C, 2013, 117, 13785-13797.	1.5	13
5772	Theoretical investigation of pressure-induced structural transitions in americium using $\langle GGA \rangle + \langle U \rangle$ and hybrid density functional theory methods. Physical Review B, 2013, 88, .	1.1	13
5773	End-Group Influence on Frontier Molecular Orbital Reorganization and Thermoelectric Properties of Molecular Junctions. Journal of Physical Chemistry Letters, 2013, 4, 3825-3833.	2.1	12
5774	Physicochemical vs. Vibrational Descriptors for Prediction of Odor Receptor Responses. Molecular Informatics, 2013, 32, 855-865.	1.4	19
5775	Assessing the Proton Affinities of N,N'-Diamidocarbenes. Journal of Organic Chemistry, 2013, 78, 10452-10458.	1.7	21

#	ARTICLE	IF	CITATIONS
5776	Crystal Engineering of Acentric Styryl Quinolinium Crystals with Strongly Hydrogen-Bonded Phenolic Anions. <i>Crystal Growth and Design</i> , 2013, 13, 5085-5091.	1.4	23
5777	Investigation of Magnetic Exchange Pathways in Heterotrinnuclear Manganese(III) Schiff Base Complexes Involving Tetrathiocyanidoplatinate(II) Bridges. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 5781-5789.	1.0	8
5778	Quantum chemical investigations on superhalogen properties of MnFn (n=1.6) nano-complexes and the consequential possibility of formation of new MnFn ⁺ Na salt species. <i>Journal of Fluorine Chemistry</i> , 2013, 146, 59-65.	0.9	14
5779	Modular Mesoionics: Understanding and Controlling Regioselectivity in 1,3-Dipolar Cycloadditions of MA ₄ nchnone Derivatives. <i>Journal of the American Chemical Society</i> , 2013, 135, 17349-17358.	6.6	58
5780	Computational Studies of the Electronic Absorption Spectrum of [(2,2',6',6'-Terpyridine) ²⁺ Pt(II) ⁺ OH] ⁻ [7,7,8,8-Tetracyanoquinodimethane] Complex. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12363-12373.	1.1	3
5781	Accurate Computation of Cohesive Energies for Small to Medium-Sized Gold Clusters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1964-1970.	2.3	39
5782	Accurate Surface Chemistry beyond the Generalized Gradient Approximation: Illustrations for Graphene Adatoms. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4853-4859.	2.3	20
5783	Novel Carbazole-Phenothiazine Dyads for Dye-Sensitized Solar Cells: A Combined Experimental and Theoretical Study. <i>ACS Applied Materials & Interfaces</i> , 2013, 5, 9635-9647.	4.0	102
5784	First Principle Study of Capping Energies and Electronic States in Stoichiometric and Nonstoichiometric PbSe Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2013, 117, 26396-26404.	1.5	4
5785	Hydroxo ⁺ Rhodium ⁺ N-Heterocyclic Carbene Complexes as Efficient Catalyst Precursors for Alkyne Hydrothiolation. <i>ACS Catalysis</i> , 2013, 3, 2910-2919.	5.5	53
5786	Thermochemistry of 1-Methylnaphthalene Hydroconversion: Comparison of Group Contribution and ab Initio Models. <i>Energy & Fuels</i> , 2013, 27, 5475-5482.	2.5	3
5787	Probing Heme Vibrational Anisotropy: An Imidazole Orientation Effect?. <i>Inorganic Chemistry</i> , 2013, 52, 11361-11369.	1.9	10
5788	Two Rare-Class Tricyclic Diterpenes with Antitubercular Activity from the Caribbean Sponge <i>Svenzea flava</i> . Application of Vibrational Circular Dichroism Spectroscopy for Determining Absolute Configuration. <i>Journal of Organic Chemistry</i> , 2013, 78, 11294-11301.	1.7	27
5790	Modeling the effect of ionic additives on the optical and electronic properties of a dye-sensitized TiO ₂ heterointerface: absorption, charge injection and aggregation. <i>Journal of Materials Chemistry A</i> , 2013, 1, 14675.	5.2	41
5791	Long lived charge separation in iridium(III)-photosensitized polyoxometalates: synthesis, photophysical and computational studies of organometallic ⁺ redox tunable oxide assemblies. <i>Chemical Science</i> , 2013, 4, 1737.	3.7	75
5792	Dihydrogen Phosphate as a Hydrogen-Bonding Donor Element: Anion Receptors Based on Acylhydrazones. <i>Journal of Organic Chemistry</i> , 2013, 78, 12121-12127.	1.7	16
5793	Study of geometry and electronic structure of molecules, cation-radicals, and anion-radicals of nitromethane, dimethylnitramine, and ethyl nitrate. <i>Russian Journal of General Chemistry</i> , 2013, 83, 1823-1839.	0.3	2
5794	SPECTROSCOPIC STUDY, NLO PROPERTIES AND HOMO ⁺ LUMO ANALYSIS ON DIFFERENT DONOR AND ACCEPTOR SUBSTITUENTS OF THIAZOLYLAZOPYRIMIDINE CHROMOPHORES. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350039.	1.8	3

#	ARTICLE	IF	CITATIONS
5795	Density-matrix functionals from Green's functions. <i>Physical Review B</i> , 2013, 88, .	1.1	27
5796	Defect identification in semiconductors with positron annihilation: Experiment and theory. <i>Reviews of Modern Physics</i> , 2013, 85, 1583-1631.	16.4	600
5797	Influence of added elements on autocatalytic chemical deposition electroless NiP. <i>Electrochimica Acta</i> , 2013, 114, 805-812.	2.6	22
5798	[Cp ₂ Zr(CH ₂ CHMe(SiMe ₃) ₃)] ⁺ , an Alkyl- Titanium Complex Which (a) Exists in Equilibrium between a ¹² -Agostic and a Lower Energy ¹³ -Agostic Isomer and (b) Undergoes Hydrogen Atom Exchange between ^{1±} , ¹² -, and ¹³ -Sites via a Combination of Conventional ¹² -Hydrogen Elimination Reinsertion and a Nonconventional CH Bond Activation Process Which Involves Proton Tunneling. <i>Journal of the American Chemical Society</i> , 2013, 135, 17514-17527.	6.6	21
5799	Brønsted Acid Catalyzed Enantioselective Indole Aza-Claisen Rearrangement Mediated by an Arene CH ^δ -O Interaction. <i>Journal of the American Chemical Society</i> , 2013, 135, 16380-16383.	6.6	80
5800	Transport Properties of Molecular Junctions. <i>Springer Tracts in Modern Physics</i> , 2013, , .	0.1	22
5801	A quantum chemical perspective on (6-4) photolesion repair by photolyases. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19957.	1.3	22
5802	Magnetic properties of Co ₂ TMxC and Co ₃ TMxC nanoparticles. <i>Journal of Applied Physics</i> , 2013, 114, 243909.	1.1	7
5803	5-Aminotetrazole induces spin crossover in iron(III) pentadentate Schiff base complexes: experimental and theoretical investigations. <i>Dalton Transactions</i> , 2013, 42, 16279.	1.6	13
5804	Quantum chemical studies and molecular modeling of the effect of polyethylene glycol as corrosion inhibitors of an aluminum surface. <i>Canadian Journal of Chemistry</i> , 2013, 91, 283-291.	0.6	18
5805	On the Photophysics of Carotenoids: A Multireference DFT Study of Peridinin. <i>Journal of Physical Chemistry B</i> , 2013, 117, 13808-13815.	1.2	48
5806	Immobilization and Characterization of RuCl ₂ (PPh ₃) ₃ Mesoporous Silica SBA-3. <i>Zeitschrift Fur Physikalische Chemie</i> , 2013, 227, 901-915.	1.4	7
5807	Density-Dependent Onset of the Long-Range Exchange: A Key to Donor-Acceptor Properties. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11580-11586.	1.1	26
5808	A comparative DFT study on aquation and nucleobase binding of ruthenium (II) and osmium (II) arene complexes. <i>Journal of Molecular Modeling</i> , 2013, 19, 4849-4856.	0.8	5
5809	Triphenylamine-Benzimidazole Derivatives: Synthesis, Excited-State Characterization, and DFT Studies. <i>Journal of Organic Chemistry</i> , 2013, 78, 11389-11395.	1.7	48
5810	Theoretical Prediction of XRgCO ⁺ Ions (X = F, Cl, and Rg = Ar, Kr, Xe). <i>Journal of Physical Chemistry A</i> , 2013, 117, 14282-14292.	1.1	31
5811	Donor-acceptor-donor thienyl/bithienyl-benzothiadiazole/quinoxaline model oligomers: experimental and theoretical studies. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15204.	1.3	53
5812	Novel Thiophene-Phenylene-Thiophene Fused Bis lactam-Based Donor-Acceptor Type Conjugate Polymers: Synthesis by Direct Arylation and Properties. <i>Macromolecules</i> , 2013, 46, 9220-9230.	2.2	41

#	ARTICLE	IF	CITATIONS
5813	Redox-Linked Conformational Control of Proton-Coupled Electron Transfer: Y122 in the Ribonucleotide Reductase β 2 Subunit. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8457-8468.	1.2	18
5814	Adsorption sensitivity of zigzag GeC nanotube towards N ₂ , CO, SO ₂ , HCN, NH ₃ , and H ₂ CO molecules. <i>Chemical Physics Letters</i> , 2013, 577, 107-113.	1.2	18
5815	A scaling PNO-MP2 method using a hybrid OSV-PNO approach with an iterative direct generation of OSVs. <i>Molecular Physics</i> , 2013, 111, 2463-2476.	0.8	60
5816	TD-DFT accuracy in determining excited-state structures and fluorescence spectra of firefly emitter. <i>Chemical Research in Chinese Universities</i> , 2013, 29, 982-985.	1.3	4
5817	Constrained-DFT method for accurate energy-level alignment of metal/molecule interfaces. <i>Physical Review B</i> , 2013, 88, .	1.1	54
5818	Donor-Substituted Nitrocyclopropanes: Immediate Ring-Enlargement to Cyclic Nitronates. <i>Organic Letters</i> , 2013, 15, 6098-6101.	2.4	73
5819	Exploring the limits of redox non-innocence: pseudo square planar [⁴ Me ₂ C(CH ₂ Ni(CH ₂ py) ₂)Ni] _n (n = 2+). <i>J. Electroanal. Chem.</i> 2013, 700, 1-10.	3.7	27
5820	Grid-free powder averages: On the applications of the Fokker-Planck equation to solid state NMR. <i>Journal of Magnetic Resonance</i> , 2013, 235, 121-129.	1.2	19
5821	Raman Spectroscopic Study of Temperature and Pressure Effects on the Ionic Liquid Propylammonium Nitrate. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10905-10912.	1.2	29
5822	Theoretical investigation on the kinetics and branching ratio of the gas phase reaction of sevoflurane with Cl atom. <i>Journal of Molecular Modeling</i> , 2013, 19, 4815-4822.	0.8	13
5823	Simulation of nanodrug by theoretical approach. <i>Journal of Nanostructure in Chemistry</i> , 2013, 3, 1.	5.3	18
5824	Does the environment around the H-cluster allow coordination of the pendant amine to the catalytic iron center in [FeFe]-hydrogenases? Answers from theory. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 693-700.	1.1	11
5825	Reversal of the Stereochemical Course of 1-Methyl-5-cis-Benzyl-(2-fluoromethyl)-3-dimethylimidazolidin-4-one as Catalysts in a Puzzling Fluorine Effect. <i>Helvetica Chimica Acta</i> , 2013, 96, 1815-1821.	4.4	8
5826	Structures of <i>a</i> _n [*] Ions Derived from Protonated Pentaglycine and Pentaalanine: Results from IRMPD Spectroscopy and DFT Calculations. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 1957-1968.	1.2	13
5827	Theoretical studies on the mechanism of activation of phosphoprotein phosphatases and purple acid phosphatases suggest an evolutionary strategy to survive in acidic environments. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 1019-1026.	1.1	6
5828	TD-DFT study of the for coumarins. <i>Chemical Physics Letters</i> , 2013, 583, 218-221.	1.2	19
5829	Ab initio Studies of Structural and Electronic Properties. , 2013, , 21-73.		1
5830	¹²⁹ Xe NMR chemical shift in Xe@C ₆₀ calculated at experimental conditions: Essential role of the relativity, dynamics, and explicit solvent. <i>Journal of Computational Chemistry</i> , 2013, 34, 1890-1898.	1.5	17

#	ARTICLE	IF	CITATIONS
5831	Mechanism and Enantioselectivity in Palladium-Catalyzed Conjugate Addition of Arylboronic Acids to β^2 -Substituted Cyclic Enones: Insights from Computation and Experiment. <i>Journal of the American Chemical Society</i> , 2013, 135, 14996-15007.	6.6	131
5832	Side Chain Flexibility in Perfluorosulfonic Acid Ionomers: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10534-10543.	1.1	13
5833	Toward Reliable Prediction of the Energy Ladder in Multichromophoric Systems: A Benchmark Study on the FMO Light-Harvesting Complex. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4928-4938.	2.3	52
5834	Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: The vertical transition approximation. <i>Journal of Chemical Physics</i> , 2013, 139, 114102.	1.2	36
5835	Formation of Sâ€‘Cl Phosphorothioate Adduct Radicals in dsDNA S-Oligomers: Hole Transfer to Guanine vs Disulfide Anion Radical Formation. <i>Journal of the American Chemical Society</i> , 2013, 135, 12827-12838.	6.6	27
5836	Weight Loss, Electrochemical, Quantum Chemical Calculation, and Molecular Dynamics Simulation Studies on 2-(Benzylthio)-1,4,5-triphenyl-1H-imidazole as an Inhibitor for Carbon Steel Corrosion in Hydrochloric Acid. <i>Industrial & Engineering Chemistry Research</i> , 2013, 52, 14315-14327.	1.8	71
5837	p-Nitrophenyl Ethylthioester in Enantioselective Organocatalytic Michael Additions: Different Behaviour of β^2 -Aryl and β^2 -Alkyl Enals. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 7067-7075.	1.2	16
5838	Theoretical study on the mechanism of selective Câˆ’F bond activation of perfluorinated toluene promoted by Co(PMe ₃) ₄ . <i>Computational and Theoretical Chemistry</i> , 2013, 1018, 115-119.	1.1	4
5839	Synthesis and Electronic Structure of Dissymmetrical, Naphthalene-Bridged Sandwich Complexes [Cpâ€‘ ² Fe(β^2 -C ₁₀ H ₈)MCP*] ^x (x = 0, +1; M = Fe, Ru; Cpâ€‘ ² = 1,1’-ETQq _{0,0,0} rgBT/C	1.1	16
5840	Propagation and termination steps in Rh-mediated carbene polymerisation using diazomethane. <i>Dalton Transactions</i> , 2013, 42, 4139.	1.6	11
5841	Nuclear spin-induced Cotton-Mouton effect in molecules. <i>Journal of Chemical Physics</i> , 2013, 138, 204110.	1.2	19
5842	Brazilwood Reds: The (Photo)Chemistry of Brazilin and Brazilein. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10650-10660.	1.1	28
5843	Dissociative Photoionization of Glycerol and its Dimer Occurs Predominantly via a Ternary Hydrogen-Bridged Ionâ€‘Molecule Complex. <i>Journal of the American Chemical Society</i> , 2013, 135, 14229-14239.	6.6	37
5844	Mechanistic Basis for High Stereoselectivity and Broad Substrate Scope in the (salen)Co(III)-Catalyzed Hydrolytic Kinetic Resolution. <i>Journal of the American Chemical Society</i> , 2013, 135, 15595-15608.	6.6	115
5845	Modeling of Fluorescence Quenching by Lutein in the Plant Light-Harvesting Complex LHCII. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10974-10986.	1.2	69
5846	Ab Initio Study of the Vibrational Signatures for the Covalent Functionalization of Graphene. <i>Journal of Physical Chemistry C</i> , 0, , 130917155202007.	1.5	5
5847	Controlling Physical Properties of Iron Nanoparticles during Assembly by â€‘Click Chemistryâ€‘. <i>Journal of Physical Chemistry C</i> , 2013, 117, 19974-19983.	1.5	12
5848	Cationic cyanine dyes: impact of symmetry-breaking on optical absorption and third-order polarizabilities. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19465.	1.3	20

#	ARTICLE	IF	CITATIONS
5849	Theoretical and Experimental Analysis of the Reaction Mechanism of MrTPS2, a Triquinane-Forming Sesquiterpene Synthase from Chamomile. <i>Chemistry - A European Journal</i> , 2013, 19, 13590-13600.	1.7	30
5850	What Controls Regiochemistry in 1,3-Dipolar Cycloadditions of $M\frac{1}{4}n$ chones with Nitrostyrenes?. <i>Organic Letters</i> , 2013, 15, 5218-5221.	2.4	47
5851	Space group symmetry applied to SCF calculations with periodic boundary conditions and Gaussian orbitals. <i>Journal of Chemical Physics</i> , 2013, 139, 114110.	1.2	5
5852	Quantum Chemical Study of the Enzymatic Repair of T(6)C/C(6)T UV-Photolesions by DNA Photolyases. <i>ChemPhysChem</i> , 2013, 14, 2817-2824.	1.0	8
5853	Quantifying the Nature of Lone Pair Domains. <i>ChemPhysChem</i> , 2013, 14, 3714-3725.	1.0	28
5854	Palladium Supported Catalysts for Nitrocyclohexane Hydrogenation to Cyclohexanone Oxime with High Selectivity. <i>ChemCatChem</i> , 2013, 5, 2932-2938.	1.8	12
5855	Theoretical determination of spin Hamiltonians with isotropic and anisotropic magnetic interactions in transition metal and lanthanide complexes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18784.	1.3	45
5856	All-Metal Clusters that Mimic the Chemistry of Halogens. <i>ChemPhysChem</i> , 2013, 14, 3227-3232.	1.0	9
5857	Electric response properties of neutral and charged $Al13X$ ($X=Li, Na, K$) magic clusters. A comprehensive ab initio and density functional comparative study. <i>Computational and Theoretical Chemistry</i> , 2013, 1021, 114-123.	1.1	22
5858	Double-hybrid density functionals: merging wavefunction and density approaches to get the best of both worlds. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14581.	1.3	100
5859	Computational study on the reaction of atomic chlorine with 1,2-dibromoethane (CH_2BrCH_2Br). <i>Canadian Journal of Chemistry</i> , 2013, 91, 1123-1129.	0.6	6
5860	An assessment of DFT methods for predicting the thermochemistry of ion-molecule reactions of group 14 elements (Si, Ge, Sn). <i>Journal of Molecular Modeling</i> , 2013, 19, 5439-5444.	0.8	7
5861	Electronic and Structural Properties of Neutral, Anionic, and Cationic $Rh_x Cu_{4-x}$ ($x=0-4$) Small Clusters: A DFT Study. <i>Journal of Cluster Science</i> , 2013, 24, 273-287.	1.7	25
5862	A model theoretical study on ligand exchange reactions of CoA. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6139.	1.3	2
5863	Hydrothermal synthesis of an ortho-metallated Co(III) complex anchored by a carboxylate group with a selective oxidation catalytic property. <i>Dalton Transactions</i> , 2013, 42, 4313.	1.6	5
5864	π - $H\cdots\pi$ interactions as modulators of carbocation structure – implications for terpene biosynthesis. <i>Chemical Science</i> , 2013, 4, 2512.	3.7	45
5865	Benchmark Study of the Performance of Density Functional Theory for Bond Activations with (Ni,Pd)-Based Transition-Metal Catalysts. <i>ChemistryOpen</i> , 2013, 2, 115-124.	0.9	146
5866	<i>In situ</i> parameterisation of SCC-DFTB repulsive potentials by iterative Boltzmann inversion. <i>Molecular Physics</i> , 2013, 111, 3595-3607.	0.8	28

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5867	Interaction of TiO ⁺ with water: infrared photodissociation spectroscopy and density functional calculations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17126.	1.3	18
5868	Computational Hammett analysis of redox based oxy-insertion by Pt(II) complexes. <i>Dalton Transactions</i> , 2013, 42, 4114-4121.	1.6	4
5869	Fluorine-doped BP 2000: highly efficient metal-free electrocatalysts for acidic oxygen reduction reaction with superlow H ₂ O ₂ yield. <i>Chemical Communications</i> , 2013, 49, 10296.	2.2	50
5870	Magnetic properties and energy-mapping analysis. <i>Dalton Transactions</i> , 2013, 42, 823-853.	1.6	316
5871	Structural and electrochemical aspects of tris(ferrocenyl/phenyl-ethynyl)phosphine ligated chalcogen bridged iron carbonyl clusters. <i>RSC Advances</i> , 2013, 3, 26025.	1.7	11
5872	The interactions of methyl tert-butyl ether on high silica zeolites: a combined experimental and computational study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13275.	1.3	27
5873	Ultrafast branching in the excited state of coumarin and umbelliferone. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17846.	1.3	48
5874	Asymmetric niobium guanidines as intermediates in the catalytic guanylation of amines. <i>Dalton Transactions</i> , 2013, 42, 8223.	1.6	28
5875	Protection of HeLa cells against ROS stress by CuZnSOD mimic system. <i>Journal of Materials Chemistry B</i> , 2013, 1, 6042.	2.9	10
5876	Extended Lagrangian Born-Oppenheimer molecular dynamics in the limit of vanishing self-consistent field optimization. <i>Journal of Chemical Physics</i> , 2013, 139, 214102.	1.2	16
5877	A Molecular Dynamics and Quantum Mechanics/Molecular Mechanics Study of the Catalytic Reductase Mechanism of Methionine Sulfoxide Reductase A: Formation and Reduction of a Sulfenic Acid. <i>Biochemistry</i> , 2013, 52, 1814-1827.	1.2	13
5878	Wagging the Tail: Essential Role of Substrate Flexibility in FAAH Catalysis. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1202-1213.	2.3	24
5879	On the method-dependence of transition state asynchronicity in Diels-Alder reactions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5108.	1.3	76
5880	Intramolecular acid-base and coordination properties towards Na ⁺ and Mg ²⁺ of myo-inositol 1,3,4,5,6-pentakisphosphate: a structural approach to biologically relevant species. <i>Dalton Transactions</i> , 2013, 42, 6021-6032.	1.6	9
5881	Photo-isomerisation of alkenyl complexes of platinum(II): structural, spectroscopic, kinetic and computational investigations. <i>Dalton Transactions</i> , 2013, 42, 6840.	1.6	2
5882	Theoretical study on the photophysical properties of chiral mononuclear and dinuclear zinc complexes. <i>RSC Advances</i> , 2013, 3, 2241-2247.	1.7	10
5883	Polypyrrole derivatives as solvent vapor sensors. <i>RSC Advances</i> , 2013, 3, 20545.	1.7	6
5884	Syntheses and structures of eight-semi-coordinate M(II) (M=Mn, Fe, Co, Ni, Cu, Zn) complexes and density functional theory study of bond dissociation energies for the MO semi coordinate bonds. <i>Inorganic Chemistry Communication</i> , 2013, 27, 114-118.	1.8	8

#	ARTICLE	IF	CITATIONS
5885	Oxoferryl species in mononuclear non-heme iron enzymes: Biosynthesis, properties and reactivity from a theoretical perspective. <i>Coordination Chemistry Reviews</i> , 2013, 257, 277-289.	9.5	39
5886	Electronic structure of [Ni(II)S ₄] complexes from S K-edge X-ray absorption spectroscopy. <i>Coordination Chemistry Reviews</i> , 2013, 257, 564-578.	9.5	33
5887	How to design more efficient organic dyes for dye-sensitized solar cells? Adding more sp ² -hybridized nitrogen in the triphenylamine donor. <i>Journal of Power Sources</i> , 2013, 223, 86-93.	4.0	91
5888	Origin and Nature of Bond Rotation Barriers: A Unified View. <i>Journal of Physical Chemistry A</i> , 2013, 117, 962-965.	1.1	91
5889	Modeling Excited States and Alignment of Energy Levels in Dye-Sensitized Solar Cells: Successes, Failures, and Challenges. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3685-3700.	1.5	137
5890	Theoretical Study on the Regioselectivity of Baeyer-Villiger Reaction of α -Me-, -F-, -CF ₃ -Cyclohexanones. <i>Journal of Organic Chemistry</i> , 2013, 78, 146-153.	1.7	21
5891	Functional group dependence of the acid catalyzed ring opening of biomass derived furan rings: an experimental and theoretical study. <i>Catalysis Science and Technology</i> , 2013, 3, 106-115.	2.1	51
5892	Electronic Rearrangements during the Inversion of Lead Phthalocyanine. <i>Journal of Physical Chemistry A</i> , 2013, 117, 481-488.	1.1	16
5893	Chiroptical, linear, and second-order nonlinear optical properties of tetrathiafulvalenylallene: a multifunctional molecular material. <i>Journal of Materials Chemistry C</i> , 2013, 1, 1399.	2.7	23
5894	Benchmarking the Starting Points of the <i>GW</i> Approximation for Molecules. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 324-329.	2.3	206
5895	Variable Pathways for Oxygen Atom Insertion into Metal-Carbon Bonds: The Case of Cp [*] W(O) ₂ (CH ₂) ₂ SiMe ₃ . <i>Journal of the American Chemical Society</i> , 2013, 135, 424-435.	6.6	28
5896	Copper coordination to the prion protein: Insights from theoretical studies. <i>Coordination Chemistry Reviews</i> , 2013, 257, 429-444.	9.5	32
5897	Reply to "Comment on "How the Number and Location of Lithium Atoms Affect the First Hyperpolarizability of Graphene". <i>Journal of Physical Chemistry C</i> , 2013, 117, 725-728.	1.5	1
5898	The trans effect of nitroxyl (HNO) in ferrous heme systems: Implications for soluble guanylate cyclase activation by HNO. <i>Journal of Inorganic Biochemistry</i> , 2013, 118, 179-186.	1.5	33
5899	Donor and acceptor levels of organic photovoltaic compounds from first principles. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 685-695.	1.3	36
5900	New acyclic 1,2,4-triazole-based Schiff base hydrazone: Synthesis, characterization, spectrophotometric and computational studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 105, 338-343.	2.0	19
5901	C ₂ symmetrical nickel complexes derived from α -amino amides as efficient catalysts for the enantioselective addition of dialkylzinc reagents to aldehydes. <i>Tetrahedron</i> , 2013, 69, 551-558.	1.0	18
5902	Molecular and electronic structure of triethylammonium salt of N-[(1-acetyl-2-oxopropyl)(phenyl)- λ -4-sulfanylidene]ethanesulfonamide. <i>Journal of Sulfur Chemistry</i> , 2013, 34, 421-431.	1.0	0

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5903	Ab Initio, Density Functional Theory, and Semi-Empirical Calculations. <i>Methods in Molecular Biology</i> , 2013, 924, 3-27.	0.4	6
5904	Dibenzo[<i>b,f</i>]phosphepines: Novel Phosphane-Olefin Ligands for Transition Metals. <i>Organometallics</i> , 2013, 32, 363-373.	1.1	27
5905	Interfacial States in Donor-Acceptor Organic Heterojunctions: Computational Insights into Thiophene-Oligomer/Fullerene Junctions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 533-542.	2.3	45
5906	General treatment of the multimode Jahn-Teller effect: study of fullerene cations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1252-1259.	1.3	20
5907	Hückel and Möbius Bond-Shifting Routes to Configuration Change in Dehydro[4 <i>n</i> +2]annulenes. <i>Journal of Organic Chemistry</i> , 2013, 78, 2033-2039.	1.7	3
5908	Synthesis, structure, magnetic properties and theoretical calculations of methoxy bridged dinuclear iron(III) complex with hydrazone based O,N,N-donor ligand. <i>Dalton Transactions</i> , 2013, 42, 2803-2812.	1.6	38
5909	Molecular dipole effects on tuning electron transfer in a porphine-quinone complex: a DFT and TDDFT study. <i>Journal of Molecular Modeling</i> , 2013, 19, 697-704.	0.8	10
5910	Regioselectivity in Sonogashira synthesis of 6-(4-nitrobenzyl)-2-phenylthiazolo[3,2- <i>b</i>]1,2,4-triazole: a quantum chemistry study. <i>Journal of Molecular Modeling</i> , 2013, 19, 951-961.	0.8	32
5911	Lowest triplet (π, π^*) electronic state of acrolein: Determination of structural parameters by cavity ringdown spectroscopy and quantum-chemical methods. <i>Journal of Chemical Physics</i> , 2013, 138, 064303.	1.2	6
5912	Influence of Base and Structure in the Reversible Covalent Conjugate Addition of Thiol to Polycyclic Enone Scaffolds. <i>Organic Letters</i> , 2013, 15, 1076-1079.	2.4	23
5913	Electrostatic spectral tuning mechanism of the green fluorescent protein. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4491.	1.3	47
5914	Conformational Analysis of γ -Lactones by DFT Calculations: The Parent Compound and its Monomethyl and Selected Dimethyl Derivatives. <i>Chemistry - A European Journal</i> , 2013, 19, 1288-1302.	1.7	9
5915	Crucial Influence of the Intramolecular Hydrogen Bond on the Coordination Mode of RC(S)NHP(S)(OiPr) ₂ in Homoleptic Complexes with Ni(II). <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 545-555.	1.0	17
5916	Model Suite for Predicting the Aquatic Toxicity of α, β -Unsaturated Esters Triggered by Their Chemoavailability. <i>Molecular Informatics</i> , 2013, 32, 98-107.	1.4	5
5917	Experimental and theoretical studies on protective properties of poly(pyrrole-co-N-methyl pyrrole) coatings on copper in chloride media. <i>Corrosion Science</i> , 2013, 69, 252-261.	3.0	45
5918	High reactivity of nitric oxide with peroxy groups on BaO particles. DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2013, 1009, 1-7.	1.1	1
5919	Cadinane sesquiterpenes from the mushroom <i>Lyophyllum transforme</i> . <i>Phytochemistry</i> , 2013, 93, 192-198.	1.4	6
5920	Structural, bonding, and magnetic properties of Fe _n (n, $x \approx 1/26$) clusters: Theoretical investigation based on density functional theory. <i>Computational Materials Science</i> , 2013, 68, 350-360.	1.4	4

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5921	Gas-phase collision induced dissociation mechanisms of peptides: Theoretical and experimental study of N-formylalanyl amide fragmentation. <i>International Journal of Mass Spectrometry</i> , 2013, 335, 33-44.	0.7	30
5922	Structure, stability and superhalogen properties of sodium and magnesium borohydrides. <i>Chemical Physics Letters</i> , 2013, 556, 173-177.	1.2	19
5923	Guided ion-beam and theoretical studies of the reaction of Os ⁺ (6D) with O ₂ : Adiabatic and nonadiabatic behavior. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 87-98.	0.7	25
5924	Theoretical study on the CH ₂ =NC hydrogen bond interaction in thiophene-based molecules. <i>Computational and Theoretical Chemistry</i> , 2013, 1005, 45-52.	1.1	5
5926	Theoretical and Experimental Investigation of Palladium(II)-Catalyzed Decarboxylative Addition of Arenecarboxylic Acid to Nitrile. <i>Organometallics</i> , 2013, 32, 490-497.	1.1	22
5927	Modeling Materials and Processes in Dye-Sensitized Solar Cells: Understanding the Mechanism, Improving the Efficiency. <i>Topics in Current Chemistry</i> , 2013, 352, 151-236.	4.0	24
5928	Mechanism-Based Inactivation of Cytochromes by Furan Epoxide: Unraveling the Molecular Mechanism. <i>Inorganic Chemistry</i> , 2013, 52, 13496-13508.	1.9	23
5929	Mechanistic Insights into the Rhenium-Catalyzed Alcohol-Olefin Dehydration Reaction. <i>Chemistry - A European Journal</i> , 2013, 19, 13224-13234.	1.7	37
5930	Density functional and Monte Carlo-based electron transport simulation in 4H-SiC(0001)/SiO ₂ DMOSFET transition region. , 2013, , .		1
5931	Theoretical study of the interaction of O ₂ with pure and mixed clusters of germanium and tin. <i>Computational and Theoretical Chemistry</i> , 2013, 1020, 113-120.	1.1	4
5932	Mechanism and Substrate-Dependent Rate-Determining Step in Palladium-Catalyzed Intramolecular Decarboxylative Coupling of Arenecarboxylic Acids with Aryl Bromides: A DFT Study. <i>Organometallics</i> , 2013, 32, 6957-6968.	1.1	21
5933	A DFT study on palladium-catalyzed decarboxylative intramolecular aziridination reaction mechanism. <i>Journal of Organometallic Chemistry</i> , 2013, 745-746, 417-422.	0.8	11
5934	Reduction of N ₂ by H ₂ to NH ₃ and N ₂ H ₄ using [MoL] (L=triamidoamine) and organic co-catalysts: A theoretical approach. <i>Journal of Molecular Catalysis A</i> , 2013, 370, 140-144.	4.8	14
5935	The direct syn-aldol and anti-Mannich reactions catalyzed by axially chiral amino sulfonamide and contrasts with proline catalysis: Insight from a computational study. <i>Computational and Theoretical Chemistry</i> , 2013, 1018, 77-84.	1.1	4
5936	Third-order nonlinear optical properties of molecules containing aromatic diimides: Effects of the aromatic core size and a redox-switchable modification. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 41, 79-88.	1.3	12
5937	Thermal and photochemical reactions of phenylethynyltris-(trimethylsilyl)germane. <i>Journal of Organometallic Chemistry</i> , 2013, 727, 50-59.	0.8	3
5938	Density functional theory study on the influence of pyrrolidine substituent of C ₆₀ bisadduct on its supramolecular interaction with porphine. <i>Chemical Physics</i> , 2013, 423, 43-48.	0.9	2
5939	Synthesis, spectroscopic, thermal and DFT calculations of 2-(3-amino-2-hydrazono-4-oxothiazolidin-5-yl) acetic acid binuclear metal complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 111, 169-177.	2.0	30

#	ARTICLE	IF	CITATIONS
5940	Density functional theory investigations of bismuth vanadate: Effect of hybrid functionals. <i>Computational Materials Science</i> , 2013, 74, 33-39.	1.4	28
5941	Experimental and theoretical insights into the sequential oxidations of 3i-2spiro molecules derived from oligophenylenes: A comparative study of 1,2-b-DiSpiroFluorene-IndenoFluorene versus 1,2-b-DiSpiroFluorene(tert-butyl)4-IndenoFluorene. <i>Electrochimica Acta</i> , 2013, 110, 735-740.	2.6	9
5942	A study of the valence shell electronic structure and photoionisation dynamics of para-dichlorobenzene and para-bromochlorobenzene. <i>Chemical Physics</i> , 2013, 415, 291-308.	0.9	15
5943	Stabilization of diketo tautomer of curcumin by pre-micellar anionic surfactants: UV-Visible, fluorescence, tensiometric and TD-DFT evidences. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 104, 150-157.	2.0	41
5944	ESIPT-inspired benzothiazole fluorescein: Photophysics of microenvironment pH and viscosity. <i>Dyes and Pigments</i> , 2013, 98, 507-517.	2.0	42
5945	Intramolecular cyclization reaction mechanism and regioselectivities of unsubstituted and benzene-substituted 4-penteniminy radicals: A DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2013, 1005, 75-83.	1.1	10
5946	Computational study on the molecular structures and photoelectron spectra of bimetallic oxide clusters (M=V, Nb, Ta). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 109, 125-132.	2.0	8
5947	Modeling of multifunctional donor-bridge-acceptor 4,6-di(thiophen-2-yl)pyrimidine derivatives: A first principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 44, 168-176.	1.3	30
5948	Syntheses and highly enantioselective fluorescent recognition of L±-hydroxyl/amino carboxylic acid anions in protic solutions. <i>Sensors and Actuators B: Chemical</i> , 2013, 177, 384-389.	4.0	26
5949	Complete methane-to-methanol catalytic cycle: A DFT study of oxygen atom transfer from N2O to late-row (Mn, Cu, Zn) η^2 -diketiminato CH activation catalysts. <i>Polyhedron</i> , 2013, 52, 945-956.	1.0	20
5950	Domino synthesis of protochromic ON-OFF-ON luminescent 2-styryl quinolines. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 2597.	1.5	21
5951	Benchmark Study for the Cysteine-Histidine Proton Transfer Reaction in a Protein Environment: Gas Phase, COSMO, QM/MM Approaches. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1765-1777.	2.3	41
5952	Molecular Design of Porphyrins for Dye-Sensitized Solar Cells: A DFT/TDDFT Study. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 524-530.	2.1	123
5953	Mechanistic Investigations and Secondary Coordination Sphere Effects in the Hydration of Nitriles with [Ru(<i>i</i> -6-arene)Cl ₂ PR ₃] Complexes. <i>Organometallics</i> , 2013, 32, 824-834.	1.1	50
5954	Improving the Photovoltage of Dithienopyrrole Dye-Sensitized Solar Cells via Attaching the Bulky Bis(octyloxy)biphenyl Moiety to the Conjugated Linker. <i>Advanced Functional Materials</i> , 2013, 23, 3539-3547.	7.8	70
5955	Molecular structural, non-linear optical, second order perturbation and Fukui studies of Indole-3-Aldehyde using density functional calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 106, 299-309.	2.0	27
5956	Iron in a Trigonal Tris(alkoxide) Ligand Environment. <i>Inorganic Chemistry</i> , 2013, 52, 3159-3169.	1.9	30
5957	Analysis of double-hybrid density functionals along the adiabatic connection. <i>Molecular Physics</i> , 2013, 111, 1275-1294.	0.8	42

#	ARTICLE	IF	CITATIONS
5958	Gas-Phase Reactions Regarding GaN Crystal Growth in a Carbon-Based Transport System: A Quantum Chemical Study. <i>Crystal Growth and Design</i> , 2013, 13, 1445-1457.	1.4	5
5959	Efficient and Accurate Theoretical Methods To Investigate Anion- π Interactions in Protein Model Structures. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3315-3322.	1.2	26
5960	DFT based approach to photophysical properties. <i>Tetrahedron</i> , 2013, 69, 1767-1777.	1.0	41
5961	Photophysical properties of azaboradibenzo[6]helicene derivatives. <i>Journal of Materials Chemistry C</i> , 2013, 1, 2354.	2.7	27
5962	Dynamics of Single Fe Atoms in Graphene Vacancies. <i>Nano Letters</i> , 2013, 13, 1468-1475.	4.5	228
5963	Conversion of a Singlet Silylene to a stable Biradical. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 1801-1805.	7.2	167
5964	Enhancement of DFT-calculations at petascale: Nuclear Magnetic Resonance, Hybrid Density Functional Theory and Car-Parinello calculations. <i>Computer Physics Communications</i> , 2013, 184, 1827-1833.	3.0	33
5965	Accurate Reaction Energies in Proteins Obtained by Combining QM/MM and Large QM Calculations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 640-649.	2.3	80
5966	Highly regioselective opening of zirconacyclopentadienes by remote coordination: concise synthesis of the furan core of the leupyrrins. <i>Chemical Communications</i> , 2013, 49, 725-727.	2.2	14
5967	Increasing the Efficiency of the Transannular Diels-Alder Strategy via Palladium(II)-Catalyzed Macrocyclizations. <i>Organic Letters</i> , 2013, 15, 582-585.	2.4	24
5968	Heteroleptic Cu(I) Bis-diimine Complexes of 6,6'-Dimesityl-2,2'-bipyridine: A Structural, Theoretical and Spectroscopic Study. <i>Inorganic Chemistry</i> , 2013, 52, 2980-2992.	1.9	53
5969	Facile Synthesis of 2-Substituted Benzo[b]thiophen-3-ols in Water. <i>Synthetic Communications</i> , 2013, 43, 1337-1344.	1.1	6
5970	A conformational study of hydroxyflavones by vibrational spectroscopy coupled to DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 109, 116-124.	2.0	29
5971	5,6-Bis(octyloxy)benzo[1,2,5]thiadiazole-Bridged Dyes for Dye-Sensitized Solar Cells with High Open-Circuit Voltage Performance. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 1770-1780.	1.2	31
5972	Mechanistic insights into the bioactivation of phenacetin to reactive metabolites: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2013, 1007, 48-56.	1.1	20
5973	Mechanistic Investigation of Palladium-Catalyzed Allylic C-H Activation. <i>ACS Catalysis</i> , 2013, 3, 294-302.	5.5	79
5974	Torsional barriers of substituted biphenyls calculated using density functional theory: a benchmarking study. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 2859.	1.5	51
5975	Photo-assisted cyanation of transition metal nitrates coupled with room temperature C-C bond cleavage of acetonitrile. <i>Chemical Communications</i> , 2013, 49, 1906.	2.2	17

#	ARTICLE	IF	CITATIONS
5996	DFT calculations of effective exchange integrals at the complete basis set limit on oxo-vanadium ring complex. <i>Polyhedron</i> , 2013, 66, 97-101.	1.0	7
5997	PaternÅ²Å¼chi reaction versus hydrogen abstraction in the photochemical reactivity of alkenyl boronates with benzophenone. <i>Tetrahedron</i> , 2013, 69, 3782-3795.	1.0	9
5998	Intramolecular OxyallylÅ¼Carbonyl (3 + 2) Cycloadditions. <i>Journal of the American Chemical Society</i> , 2013, 135, 5242-5245.	6.6	42
5999	Synthesis and self-assembly of triphenylene-containing conjugated macrocycles. <i>RSC Advances</i> , 2013, 3, 6008.	1.7	8
6000	Gold(I)-Catalyzed Formation of Bicyclo[4.2.0]oct-1-enes. <i>Journal of Organic Chemistry</i> , 2013, 78, 5685-5690.	1.7	22
6001	Electronic and magnetic properties of double perovskite slab-rocksalt layer rare earth strontium aluminates natural superlattice structure. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	10
6002	One-Pot, Two-Step, Microwave-Assisted Palladium-Catalyzed Conversion of Aryl Alcohols to Aryl Fluorides via Aryl Nonaflates. <i>Journal of Organic Chemistry</i> , 2013, 78, 4184-4189.	1.7	34
6003	A synergistic combination of tetraethylorthosilicate and multiphosponic acid offers excellent corrosion protection to AA1100 aluminum alloy. <i>Applied Surface Science</i> , 2013, 273, 758-768.	3.1	61
6004	Subtle Å¼supramolecular buttressing effectsÅ¼in Cucurbit[7]uril/guest assemblies. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 3116.	1.5	11
6005	Molecular Mechanism of Polyacrylate Helix Sense Switching across Its Free Energy Landscape. <i>Journal of the American Chemical Society</i> , 2013, 135, 5509-5512.	6.6	65
6006	Band gaps from the Tran-Blaha modified Becke-Johnson approach: A systematic investigation. <i>Journal of Chemical Physics</i> , 2013, 138, 134115.	1.2	176
6007	Comprehensive Analysis of Fragment Orbital Interactions to Build Highly Å¼Conjugated ThienyleneÅ¼Substituted Phenylene Oligomers. <i>Chemistry - A European Journal</i> , 2013, 19, 7532-7546.	1.7	15
6008	An improved B3LYP method in the calculation of organic thermochemistry and reactivity. <i>Computational and Theoretical Chemistry</i> , 2013, 1015, 64-71.	1.1	56
6009	Structural Evidence for Undecabromide [Br₁₁]^{Å¼}. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 4937-4940.	7.2	49
6010	Cycloaddition of ozone to allyl alcohol, acrylic acid and allyl aldehyde: A comparative DFT study. <i>Chemical Physics</i> , 2013, 415, 161-167.	0.9	3
6011	Investigation of the Reaction Mechanism for the Epoxidation of Alkenes with Hydrogen Peroxide Catalyzed by a Protonated Tetranuclear Peroxotungstate with NMR Spectroscopy, Kinetics, and DFT Calculations. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 1943-1950.	1.0	15
6012	Ionic liquids based on the bis(trifluoromethylsulfonyl)imide anion for highÅ¼pressure Raman spectroscopy measurements. <i>Journal of Raman Spectroscopy</i> , 2013, 44, 481-484.	1.2	19
6013	Nickel(II) complexes with bridged polyamines. <i>Polyhedron</i> , 2013, 56, 1-8.	1.0	5

#	ARTICLE	IF	CITATIONS
6014	A molecular study of tetrakis(<i>p</i> -methoxyphenyl)porphyrin and its Zn(II) complex as discotic liquid crystals. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2287-2294.	1.0	8
6015	Labile Rhodium(I)-N-Heterocyclic Carbene Complexes. <i>Organometallics</i> , 2013, 32, 2768-2774.	1.1	21
6016	Linear and nonlinear optical properties of nucleic acid bases. <i>Chemical Physics</i> , 2013, 410, 90-98.	0.9	72
6017	The ammonium nitrate and its mechanism of decomposition in the gas phase: a theoretical study and a DFT benchmark. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10849.	1.3	43
6018	Interpretation and Application of Reaction Class Transition State Theory for Accurate Calculation of Thermokinetic Parameters Using Isodesmic Reaction Method. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3279-3291.	1.1	15
6019	Cyanide Detection Using a Triazolopyridinium Salt. <i>Organic Letters</i> , 2013, 15, 2386-2389.	2.4	79
6020	Assessing the viability of biosynthetic pathways for calophyline A formation—are pericyclic reactions involved?. <i>Tetrahedron Letters</i> , 2013, 54, 2952-2955.	0.7	6
6021	Density Functional Study of Organocatalytic Cross-Aldol Reactions between Two Aliphatic Aldehydes: Insight into Their Functional Differentiation and Origins of Chemo- and Stereoselectivities. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2862-2872.	1.1	14
6022	Sulfur(IV)-Mediated Transformations: From Ylide Transfer to Metal-Free Arylation of Carbonyl Compounds. <i>Journal of the American Chemical Society</i> , 2013, 135, 7312-7323.	6.6	137
6023	Theoretical Study of Oxygen Reduction Reaction Catalysts: From Pt to Non-precious Metal Catalysts. <i>Lecture Notes in Energy</i> , 2013, , 339-373.	0.2	2
6024	Quantum chemical study of the donor-bridge-acceptor triphenylamine based sensitizers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 110, 60-66.	2.0	73
6025	A relativistic DFT methodology for calculating the structures and NMR chemical shifts of octahedral platinum and iridium complexes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7740.	1.3	74
6026	BN Segment Doped Effect on the First Hyperpolarizability of Heteronanotubes: Focused on an Effective Connecting Pattern. <i>Journal of Physical Chemistry C</i> , 2013, 117, 10039-10044.	1.5	26
6027	Theoretical study on novel double donor-based dyes used in high efficient dye-sensitized solar cells: The application of TDDFT study to the electron injection process. <i>Organic Electronics</i> , 2013, 14, 711-722.	1.4	97
6028	Unraveling the Enigmatic Mechanism of <i>Asparaginase II</i> with QM/QM Calculations. <i>Journal of the American Chemical Society</i> , 2013, 135, 7146-7158.	6.6	57
6029	Catalytic valorization of glycerol to hydrogen and syngas. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 2678-2700.	3.8	219
6030	Research on the chelation between luteolin and Cr(III) ion through infrared spectroscopy, UV-vis spectrum and theoretical calculations. <i>Journal of Molecular Structure</i> , 2013, 1034, 386-391.	1.8	17
6031	Modification on C219 by coumarin donor toward efficient sensitizer for dye sensitized solar cells: A theoretical study. <i>Dyes and Pigments</i> , 2013, 99, 127-135.	2.0	48

#	ARTICLE	IF	CITATIONS
6032	DFT Studies on the Palladium-Catalyzed Dearomatization Reaction between Chloromethylnaphthalene and the Cyclic Amine Morpholine. <i>Organometallics</i> , 2013, 32, 2336-2343.	1.1	33
6033	Circular Dichroism of (Di)methyl- and Diaza[6]helicenes. A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 83-93.	1.1	84
6034	Theoretical study on rate constants for the reactions of CF ₃ CH ₂ NH ₂ (TFEA) with the hydroxyl radical at 298 K and atmospheric pressure. <i>Journal of Molecular Modeling</i> , 2013, 19, 2189-2195.	0.8	16
6035	Dimer radical cation of 4-thiouracil: a pulse radiolysis and theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 510-516.	0.9	11
6036	Comparative evaluation of a Pictet-Spengler protocol in microwave-assisted conversions of tryptamine with aryl- and carboxyaryl aldehydes: role of ring strain in cyclocondensation of the primarily formed carboxyaryl-substituted 1 ² -carbolines. <i>Monatshefte für Chemie</i> , 2013, 144, 1381-1387.	0.9	10
6037	Structural and magnetic characterizations of the first manganese(III) Schiff base complexes involving hexathiocyanidoplatinate(IV) bridges. <i>CrystEngComm</i> , 2013, 15, 5351.	1.3	9
6038	Bioinspired Nonheme Iron Complexes Derived from an Extended Series of N,N,O-Ligated BAIP Ligands. <i>Inorganic Chemistry</i> , 2013, 52, 7394-7410.	1.9	21
6039	Computational Investigation of the Competition between the Concerted Diels-Alder Reaction and Formation of Diradicals in Reactions of Acrylonitrile with Nonpolar Dienes. <i>Journal of Organic Chemistry</i> , 2013, 78, 6582-6592.	1.7	23
6040	Combined experimental and DFT computational studies on (E)-1-(5-nitrothiophen-2-yl)-N-[4-(trifluoromethyl)phenyl]methanimine. <i>Journal of Molecular Structure</i> , 2013, 1048, 41-50.	1.8	40
6041	Metal Ion Complexes with HisGly: Comparison with PhePhe and PheGly. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5335-5343.	1.1	31
6042	Quantum Mechanical Calculations of Xanthophyll-Chlorophyll Electronic Coupling in the Light-Harvesting Antenna of Photosystem II of Higher Plants. <i>Journal of Physical Chemistry B</i> , 2013, 117, 7605-7614.	1.2	13
6043	Efficient Methods for the Quantum Chemical Treatment of Protein Structures: The Effects of London-Dispersion and Basis-Set Incompleteness on Peptide and Water-Cluster Geometries. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3240-3251.	2.3	75
6044	Probing the Smallest Molecular Model of MoS ₂ Catalyst: S ₂ Units in the MoS _n (n = 1-5) Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5632-5641.	1.1	21
6045	Catalytic Nitrile Hydration with [Ru(1-6-p-cymene)Cl ₂ (PR ₂ R ²)] Complexes: Secondary Coordination Sphere Effects with Phosphine Oxide and Phosphinite Ligands. <i>Organometallics</i> , 2013, 32, 3744-3752.	1.1	47
6046	CsCdInQ ₃ (Q = Se, Te): New Photoconductive Compounds As Potential Materials for Hard Radiation Detection. <i>Chemistry of Materials</i> , 2013, 25, 2089-2099.	3.2	50
6047	Simulating Ru L ₃ -Edge X-ray Absorption Spectroscopy with Time-Dependent Density Functional Theory: Model Complexes and Electron Localization in Mixed-Valence Metal Dimers. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4444-4454.	1.1	59
6048	Quantum chemical investigation on the structural and electronic properties of zinc-salphen complex: DFT and QTAIM analysis. <i>Computational and Theoretical Chemistry</i> , 2013, 1004, 31-37.	1.1	18
6049	Understanding the Density Functional Dependence of DFT-Calculated Electronic Couplings in Organic Semiconductors. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 919-924.	2.1	79

#	ARTICLE	IF	CITATIONS
6050	Two-photon-induced singlet fission in rubrene single crystal. <i>Journal of Chemical Physics</i> , 2013, 138, 184508.	1.2	30
6051	A simple DFT-based diagnostic for nondynamical correlation. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	114
6052	The Periodate-Based Double Perovskites M_2NaO_6 ($M = Ca, Sr, \text{and } Tl$) <i>ETC</i> 0.0 0.0 BT /Overlo	0.8	23
6053	Synthesis and characterization of novel yellow azo dyes from 2-morpholin-4-yl-1,3-thiazol-4(5H)-one and study of their azo-hydrazone tautomerism. <i>Dyes and Pigments</i> , 2013, 99, 291-298.	2.0	37
6054	Complexes of 4-substituted phenolates with HF and HCN: Energy decomposition and electronic structure analyses of hydrogen bonding. <i>Journal of Computational Chemistry</i> , 2013, 34, 696-705.	1.5	8
6055	A combined DFT and restricted open-shell configuration interaction method including spin-orbit coupling: Application to transition metal L-edge X-ray absorption spectroscopy. <i>Journal of Chemical Physics</i> , 2013, 138, 204101.	1.2	210
6056	The effect of remote substitution on formation of preferential geometrical isomer of cobalt(III)-tetrazolato complexes formed via [2+3] cycloaddition. <i>Inorganic Chemistry Communication</i> , 2013, 34, 62-67.	1.8	10
6057	Density Functional Theory and Beyond for Band-Gap Screening: Performance for Transition-Metal Oxides and Dichalcogenides. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2950-2958.	2.3	99
6058	Alternation of Charge Injection and Recombination in Dye-Sensitized Solar Cells by the Addition of Nonconjugated Bridge to Organic Dyes. <i>Journal of Physical Chemistry C</i> , 2013, 117, 2024-2031.	1.5	33
6059	Caryolene-forming carbocation rearrangements. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 323-331.	1.3	23
6060	Insights into the Catalytic Mechanism of Coral Allene Oxide Synthase: A Dispersion Corrected Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 6701-6710.	1.2	21
6061	A Mononuclear Non-Heme High-Spin Iron(III)-Hydroperoxo Complex as an Active Oxidant in Sulfoxidation Reactions. <i>Journal of the American Chemical Society</i> , 2013, 135, 8838-8841.	6.6	71
6062	On the Metric of Charge Transfer Molecular Excitations: A Simple Chemical Descriptor. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3118-3126.	2.3	335
6063	Surface Reaction of Acetylene with H-Terminated Silicon Surfaces. A Theoretical Study from Hybrid DFT-D2 Periodic Simulations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 15130-15138.	1.5	6
6064	Is There Still Room for Parameter Free Double Hybrids? Performances of PBE0-DH and B2PLYP over Extended Benchmark Sets. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3444-3452.	2.3	37
6065	Vibrational spectra, DFT quantum chemical calculations and conformational analysis of P-iodoanisole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 113, 236-249.	2.0	2
6066	MD and QM/MM study on catalytic mechanism of a FAD-dependent enzyme ORF36: For nitro sugar biosynthesis. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 44, 9-16.	1.3	9
6067	TD-DFT Study of Excited-State Intramolecular Proton Transfer (ESIPT) of 2-(1,3-benzothiazol-2-yl)-5-(N,N-diethylamino)Phenol with Benzoxazole and Benzimidazole Analogues. <i>Procedia Computer Science</i> , 2013, 18, 797-805.	1.2	6

#	ARTICLE	IF	CITATIONS
6068	FTIR, FT-RAMAN, NMR, spectra, normal co-ordinate analysis, NBO, NLO and DFT calculation of N,N-diethyl-4-methylpiperazine-1-carboxamide molecule. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 275-286.	2.0	27
6069	Role of electronic correlation in high-low temperature phase transition of hexagonal nickel sulfide: A comparative density functional theory study with and without correction for on-site Coulomb interaction. <i>Journal of Chemical Physics</i> , 2013, 138, 244703.	1.2	13
6070	Novel silanetellones: Structures, ionization potentials, electron affinities, singlet \rightarrow triplet gaps and Kohn \rightarrow Sham HOMO \rightarrow LUMO gaps of the X ₂ SiTe and XYSiTe (X, Y=H, F, Cl, Br, I and CN) molecules. <i>Computational and Theoretical Chemistry</i> , 2013, 1016, 62-72.	1.1	6
6071	Quantum Chemical Calculations of Intramolecular Vibrational Redistribution and Energy Transfer of Dipeptides (GlyTyr and LeuTyr) and Applications to the RRKM Theory. <i>Journal of the Chinese Chemical Society</i> , 2013, 60, 974-985.	0.8	4
6072	Surface enhancement Raman scattering of tautomeric thiobarbituric acid. Natural bond orbitals and B3LYP/6-311+G (d, p) assignments of the Fourier Infrared and Fourier Raman Spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 114, 475-485.	2.0	15
6073	A simple but effective modeling strategy for structural properties of non \rightarrow heme Fe(II) sites in proteins: Test of force field models and application to proteins in the AlkB family. <i>Journal of Computational Chemistry</i> , 2013, 34, 1620-1635.	1.5	12
6074	First Principles Studies of the Vibrationally Resolved Magnetic Circular Dichroism Spectra of Biphenylene. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1557-1567.	2.3	19
6075	Pt ^{II} -Catalyzed Ethylene Hydrophenylation: Influence of Dipyriddy Chelate Ring Size on Catalyst Activity and Longevity. <i>ACS Catalysis</i> , 2013, 3, 1165-1171.	5.5	45
6076	Phenomenon of Quantum Entanglement in a System Composed of Two Minimal Protocells. <i>Origins of Life and Evolution of Biospheres</i> , 2013, 43, 49-66.	0.8	4
6077	Rare-earth mononitrides. <i>Progress in Materials Science</i> , 2013, 58, 1316-1360.	16.0	124
6078	Density functional theory and Ab initio studies of vibrational spectroscopic (FT-IR, FT-Raman and UV) first order hyperpolarizabilities, NBO, HOMO \rightarrow LUMO and TD-DFT analysis of the 1,2-Dihydropyrazolo (4,3-E) Pyrimidin-4-one. <i>Solid State Sciences</i> , 2013, 16, 45-52.	1.5	10
6079	Theoretical Study on the Acidities of Chiral Phosphoric Acids in Dimethyl Sulfoxide: Hints for Organocatalysis. <i>Journal of Organic Chemistry</i> , 2013, 78, 7076-7085.	1.7	106
6080	A two-dimensional photoluminescent cadmium(II) coordination polymer containing a new coordination mode of pyridine-2,3-dicarboxylate: Synthesis, structure and molecular simulations for gas storage and separation applications. <i>Polyhedron</i> , 2013, 50, 314-320.	1.0	41
6081	Excited States of Large Open-Shell Molecules: An Efficient, General, and Spin-Adapted Approach Based on a Restricted Open-Shell Ground State Wave function. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3069-3083.	1.1	81
6082	New tris-3,4-HOPO lanthanide complexes as potential imaging probes: complex stability and magnetic properties. <i>Dalton Transactions</i> , 2013, 42, 6046.	1.6	28
6083	<i>cis</i> \rightarrow <i>trans</i> Amide Bond Rotamers in β -Peptoids and Peptoids: Evaluation of Stereoelectronic Effects in Backbone and Side Chains. <i>Journal of the American Chemical Society</i> , 2013, 135, 2835-2844.	6.6	122
6084	Unexpected isomerization of new naphth[1,3]oxazino[2,3-a]isoquinolines in solution, studied by dynamic NMR and supported by theoretical DFT computations. <i>Tetrahedron</i> , 2013, 69, 7455-7465.	1.0	17
6085	Effects of substituents on the formation of rhenium carbyne and β -vinyl complexes from the reactions of ReH ₅ (PMe ₂ Ph) ₃ with terminal alkynes. <i>New Journal of Chemistry</i> , 2013, 37, 1823.	1.4	17

#	ARTICLE	IF	CITATIONS
6086	Mechanistic comparison of saccharide depolymerization catalyzed by dicarboxylic acids and glycosidases. <i>RSC Advances</i> , 2013, 3, 9273.	1.7	11
6087	Oxygen Defects and Surface Chemistry of Ceria: Quantum Chemical Studies Compared to Experiment. <i>Chemical Reviews</i> , 2013, 113, 3949-3985.	23.0	849
6088	Organic sensitizers incorporating 3,4-ethylenedioxythiophene as the conjugated bridge: Joint photophysical and electrochemical analysis of photovoltaic performance. <i>Dyes and Pigments</i> , 2013, 99, 176-184.	2.0	17
6089	Half sandwich complexes of chalcogenated pyridine based bi-(N, S/Se) and terdentate (N, S/Se, N) ligands with (1-6-benzene)ruthenium(II): synthesis, structure and catalysis of transfer hydrogenation of ketones and oxidation of alcohols. <i>Dalton Transactions</i> , 2013, 42, 8736.	1.6	38
6090	Chiral Hexa- and Nonamethylene-Bridged Bis(L-Leu-Oxalamide) Gelators: The First Oxalamide Gels Containing Aggregates with a Chiral Morphology. <i>Chemistry - A European Journal</i> , 2013, 19, 8558-8572.	1.7	17
6091	Cytochrome P450 compound I in the plane wave pseudopotential framework: GGA electronic and geometric structure of thiolate-ligated iron(IV)-oxo porphyrin. <i>Journal of Computational Chemistry</i> , 2013, 34, 1647-1660.	1.5	3
6092	Thermochemical Properties of Methyl-Substituted Cyclic Alkyl Ethers and Radicals for Oxiranes, Oxetanes, and Oxolanes: C-H Bond Dissociation Enthalpy Trends with Ring Size and Ether Site. <i>Journal of Physical Chemistry A</i> , 2013, 117, 378-392.	1.1	19
6093	Synthesis, characterization and density functional theory investigations of the electronic, photophysical and charge transfer properties of donor-bridge-acceptor triaminopyrazolo[1,5-a]pyrimidine dyes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 111, 223-229.	2.0	36
6094	Photodynamics of Schiff Base Salicylideneaniline: Trajectory Surface-Hopping Simulations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4574-4583.	1.1	78
6095	Nuclear magnetic resonance predictions for graphenes: concentric finite models and extrapolation to large systems. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4634.	1.3	26
6096	Structural Diversity from the Transannular Cyclizations of Natural Germacrone and Epoxy Derivatives: A Theoretical-Experimental Study. <i>Chemistry - A European Journal</i> , 2013, 19, 6598-6612.	1.7	21
6097	Which density functional is close to CCSD accuracy to describe geometry and interaction energy of small noncovalent dimers? A benchmark study using Gaussian09. <i>Journal of Computational Chemistry</i> , 2013, 34, 1341-1353.	1.5	108
6098	Probing the Electronic Properties of W_3O_{10} ($x=0$) ($x=1$) Tj ETQq0.0.0 rgBT /Overlock W_3O_{10} . <i>Journal of Physical Chemistry A</i> , 2013, 117, 3093-3099.	1.1	16
6099	A bond, ring and cage resolved Poincaré-Hopf relationship for isomerisation reaction pathways. <i>Molecular Physics</i> , 2013, 111, 3104-3116.	0.8	17
6100	Effects of Mn doping on $(TiO_2)_n$ ($n=2-5$) complexes. <i>Computational and Theoretical Chemistry</i> , 2013, 1013, 32-45.	1.1	15
6101	Pyrenoimidazole-Based Deep-Blue-Emitting Materials: Optical, Electrochemical, and Electroluminescent Characteristics. <i>Chemistry - an Asian Journal</i> , 2013, 8, 2111-2124.	1.7	53
6102	Structure-Property Relationship and Chemical Aspects of Oxide-Metal Hybrid Nanostructures. <i>Chemical Reviews</i> , 2013, 113, 4314-4372.	23.0	160
6103	Ab initio calculations and validation of the pH-dependent structures of the His37-Trp41 quartet, the heart of acid activation and proton conductance in the M2 protein of Influenza A virus. <i>Chemical Science</i> , 2013, 4, 2776.	3.7	21

#	ARTICLE	IF	CITATIONS
6104	Exploring structural requirements of aurone derivatives as antimalarials by validated DFT-based QSAR, HQSAR, and COMFAâ€“COMSIA approach. <i>Medicinal Chemistry Research</i> , 2013, 22, 6029-6045.	1.1	22
6105	Enhanced Electron-Transfer Reactivity of Nonheme Manganese(IV)â€“Oxo Complexes by Binding Scandium Ions. <i>Journal of the American Chemical Society</i> , 2013, 135, 9186-9194.	6.6	131
6106	Activation of Câ€“H bond in methane by Pd atom from the bonding evolution theory perspective. <i>Journal of Computational Chemistry</i> , 2013, 34, 1917-1924.	1.5	15
6107	Theoretical and Experimental Studies of Circular Dichroism of Mono- and Diazo[6]helicenes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5082-5092.	1.1	49
6108	TD-DFT benchmarks: A review. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2019-2039.	1.0	938
6109	Electronic Structure and Biologically Relevant Reactivity of Low-Spin {FeNO}⁸ Porphyrin Model Complexes: New Insight from a Bis-Picket Fence Porphyrin. <i>Inorganic Chemistry</i> , 2013, 52, 7766-7780.	1.9	105
6110	MM/QM study: Interactions of copper(II) and mercury(II) with food dyes in aqueous solutions. <i>International Journal of Chemical and Analytical Science</i> , 2013, 4, 49-56.	0.5	3
6111	DFT studies of structure and vibrational spectra of 4-benzylidene-1-phenyl-2-selenomorpholino-1H-imidazol-5(4H)-one and its derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 110, 333-342.	2.0	7
6112	RPF101, a new capsaicin-like analogue, disrupts the microtubule network accompanied by arrest in the G2/M phase, inducing apoptosis and mitotic catastrophe in the MCF-7 breast cancer cells. <i>Toxicology and Applied Pharmacology</i> , 2013, 266, 385-398.	1.3	37
6113	Opposing Auxiliary Conformations Produce the Same Torquoselectivity in an Oxazolidinone-Directed Nazarov Cyclization. <i>Journal of the American Chemical Society</i> , 2013, 135, 9156-9163.	6.6	43
6114	Mechanistic studies of ammonia borane dehydrogenation. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 169-179.	3.8	60
6115	Evaluation of Approximate Exchange-Correlation Functionals in Predicting One-Bond ³¹Pâ€“¹H NMR Indirect Spinâ€“Spin Coupling Constants. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1443-1451.	2.3	13
6116	Ditopic Ambiphilicity of an Anionic Dimetalloborylene Complex. <i>Journal of the American Chemical Society</i> , 2013, 135, 2313-2320.	6.6	47
6117	Structural, electronic, and magnetic properties of the europium chalcogenides: A hybrid-functional DFT study. <i>Physical Review B</i> , 2013, 88, .	1.1	16
6118	Deciphering the Photophysical Role of Conjugated Diyne in Butadiynyl Fluorophores: Synthesis, Photophysical and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6548-6560.	1.1	32
6119	Decarboxylative Palladium(II)â€“Catalyzed Synthesis of Aryl Amidines from Aryl Carboxylic Acids: Development and Mechanistic Investigation. <i>Chemistry - A European Journal</i> , 2013, 19, 13803-13810.	1.7	34
6120	Hydrogenation of Dimethyl Carbonate to Methanol by <i>trans</i> -[Ru(H)₂(PNN)(CO)] Catalysts: DFT Evidence for Ion-Pair-Mediated Metathesis Paths for Câ€“OMe Bond Cleavage. <i>Organometallics</i> , 2013, 32, 6969-6985.	1.1	49
6121	Metal Ion Binding by a G-2 Poly(ethylene imine) Dendrimer. Ion-Directed Self-Assembling of Hierarchical Mono- and Two-Dimensional Nanostructured Materials. <i>Inorganic Chemistry</i> , 2013, 52, 2125-2137.	1.9	27

#	ARTICLE	IF	CITATIONS
6122	Ultrafast spectroscopy of linear carbon chains: the case of dinaphthylpolyynes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9384.	1.3	15
6123	Methemoglobin Generation by 8-Aminoquinolines: Effect of Substitution at 5-Position of Primaquine. <i>Chemical Research in Toxicology</i> , 2013, 26, 1801-1809.	1.7	7
6124	How Does Catalase Release Nitric Oxide? A Computational Structure-Activity Relationship Study. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2951-2961.	2.5	7
6125	Extended Energy Divide-and-Conquer Method Based on Charge Conservation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1992-1999.	2.3	4
6126	Solvatochromism and the solvation structure of benzophenone. <i>Journal of Chemical Physics</i> , 2013, 138, 224308.	1.2	7
6127	Excitation Spectra of Large Jet-Cooled Polycyclic Aromatic Hydrocarbon Radicals: 9-Anthracenylmethyl (C ₁₅ H ₁₁) and 1-Pyrenylmethyl (C ₁₇ H ₁₁). <i>Journal of Physical Chemistry A</i> , 2013, 117, 13899-13907.	1.1	9
6128	Photoinduced charge transfer processes of zinc porphyrin derivatives for dye-sensitized solar cells. <i>Chemical Research in Chinese Universities</i> , 2013, 29, 974-981.	1.3	4
6129	Toward a Process-Based Molecular Model of SiC Membranes. 1. Development of a Reactive Force Field. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3308-3319.	1.5	39
6130	Molecular Simulations Highlight the Role of Metals in Catalysis and Inhibition of Type II Topoisomerase. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 857-862.	2.3	45
6131	Density functional theoretical study on the preferential selectivity of macrocyclic dicyclohexano-18-crown-6 for Sr ²⁺ ion over Th ⁴⁺ ion during extraction from an aqueous phase to organic phases with different dielectric constants. <i>Journal of Molecular Modeling</i> , 2013, 19, 5277-5291.	0.8	13
6132	Aryl-Substituted Unsymmetrical Benzothiadiazoles: Synthesis, Structure, and Properties. <i>Journal of Organic Chemistry</i> , 2013, 78, 12440-12452.	1.7	60
6133	Binding in Radical-Solvent Binary Complexes: Benchmark Energies and Performance of Approximate Methods. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1568-1579.	2.3	46
6134	Hydroxyl Ion Addition to One-Electron Oxidized Thymine: Unimolecular Interconversion of C5 to C6 OH-Adducts. <i>Journal of the American Chemical Society</i> , 2013, 135, 3121-3135.	6.6	42
6135	Zinc(II) Interactions with Brain-Derived Neurotrophic Factor N-Terminal Peptide Fragments: Inorganic Features and Biological Perspectives. <i>Inorganic Chemistry</i> , 2013, 52, 11075-11083.	1.9	27
6136	Large Density-Functional and Basis-Set Effects for the DMSO Reductase Catalyzed Oxo-Transfer Reaction. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1799-1807.	2.3	42
6137	Mechanistic and Computational Studies of Exocyclic Stereocontrol in the Synthesis of Bryostatin-like <i>cis</i> -2,6-Disubstituted 4-Alkylidenetetrahydropyrans by Prins Cyclization. <i>Journal of Organic Chemistry</i> , 2013, 78, 104-115.	1.7	12
6138	Assessment of Density Functional Methods for Obtaining Geometries at Conical Intersections in Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4526-4541.	2.3	63
6139	Conformational Control in the Population of the Triplet State and Photoreactivity of Nitronaphthalene Derivatives. <i>Journal of Physical Chemistry A</i> , 2013, 117, 14100-14108.	1.1	41

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6140	Enabling Forbidden Processes: Quantum and Solvation Enhancement of Nitrate Anion UV Absorption. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12868-12877.	1.1	37
6141	How Do Nucleophiles Accelerate the Reactions of Dialkylstannylene Acetals? The Effects of Adding Fluoride to Dialkoxydi-n-butylstannanes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12648-12657.	1.1	4
6142	Finite-field method with unbiased polarizable continuum model for evaluation of the second hyperpolarizability of an open-shell singlet molecule in solvents. <i>Journal of Computational Chemistry</i> , 2013, 34, 2345-2352.	1.5	1
6143	Origin of the Conformational Modulation of the ¹³ C NMR Chemical Shift of Methoxy Groups in Aromatic Natural Compounds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 661-669.	1.1	19
6144	Effect of Substituents on the Preferred Modes of One-Electron Reductive Cleavage of N-Cl and N-Br Bonds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 460-472.	1.1	22
6145	Role of Geometric Distortion and Polarization in Localizing Electronic Excitations in Conjugated Polymers. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1144-1154.	2.3	50
6146	Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1669-1675.	2.1	63
6147	To Jump or Not To Jump? ¹ H Hydrogen Atom Transfer in Post-cleavage Radical-Cation Complexes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1189-1196.	1.1	15
6148	Subnanometer-sized Pt/Sn alloy cluster catalysts for the dehydrogenation of linear alkanes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20727.	1.3	75
6149	Role Played by Isopropyl Substituents in Stabilizing the Putative Triple Bond in Ar-E-E-Ar (E = Si, Ge, Sn; Ar = C ₆ H ₃ -2,6-(C ₆ H ₃ -2,6-Pr ⁱ) ₂) ₂ and Ar*PbPbAr* [Ar* = C ₆ H ₃ -2,6-(C ₆ H ₂ -2,4,6-Pr ⁱ) ₃] ₂]. <i>Inorganic Chemistry</i> , 2013, 52, 8378-8388.	1.9	27
6150	Synthesis and Characterization of the Titanium Bisamide		

#	ARTICLE	IF	CITATIONS
6158	The effect of some triazole derivatives as inhibitors for the corrosion of mild steel in 5% hydrochloric acid. <i>Research on Chemical Intermediates</i> , 2013, 39, 3089-3103.	1.3	23
6159	Molecular features related to the binding mode of PPAR α agonists from QSAR and docking analyses. <i>SAR and QSAR in Environmental Research</i> , 2013, 24, 157-173.	1.0	7
6160	Fluorescence and Phosphorescence of Single C ₆₀ Molecules as Stimulated by a Scanning Tunneling Microscope. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 4814-4817.	7.2	22
6161	Theoretical Views on Activation of Methane Catalyzed by Hf ²⁺ and Oxidation of CO (x $\hat{1}$) by N ₂ O (x $\hat{1}$) Catalyzed by HfO ₂ ⁺ and TaO ₂ ⁺ . <i>Journal of Physical Chemistry A</i> , 2013, 117, 8843-8854.	1.1	9
6162	Structural, Electrochemical, and Spectroscopic Investigation of Acetate Bridged Dinuclear Tetrakis-Schiff Base Macrocycles of Mn and Zn. <i>Inorganic Chemistry</i> , 2013, 52, 13963-13973.	1.9	19
6163	Magnetic field-induced nuclear quadrupole coupling in atomic ¹³¹ Xe. <i>Molecular Physics</i> , 2013, 111, 1390-1400.	0.8	7
6164	Synthesis of 1,2-Dialkyl-, 1,4(5)-Dialkyl-, and 1,2,4(5)-Trialkylimidazoles via a One-Pot Method. <i>Industrial & Engineering Chemistry Research</i> , 2013, 52, 11880-11887.	1.8	19
6165	Radical-Radical Interactions among Oxidized Guanine Bases Including Guanine Radical Cation and Dehydrogenated Guanine Radicals. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10698-10710.	1.2	6
6166	Theoretical Study of Excess Electron Attachment Dynamics to the Guanine-Cytosine Base Pair: Electronic Structure Calculations and Ring-Polymer Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11403-11410.	1.1	9
6167	Electronic structures, stabilities and spectroscopic properties of Pb _m Si _n (m < i> n) (m < i> n) clusters. <i>Molecular Physics</i> , 2013, 111, 31-47.		
6168	Explaining the Temperature Dependence of Spirilloxanthin's S* Signal by an Inhomogeneous Ground State Model. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6303-6310.	1.1	22
6169	Monohafnium Oxide Clusters HfO _n ⁺ and HfO _n (< i> n = 1-6): Oxygen Radicals, Superoxides, Peroxides, Diradicals, and Triradicals. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1042-1052.	1.1	23
6170	Probing the performances of HISS functionals for the description of excited states of molecular systems. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	1
6171	Direct dynamics simulations of the hydrogen abstraction reaction Cl + CF ₃ CF ₂ CH ₂ OH. <i>Journal of Molecular Modeling</i> , 2013, 19, 4503-4510.	0.8	11
6172	TDDFT Studies on the Determination of the Absolute Configurations and Chiroptical Properties of Strandberg-Type Polyoxometalates. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2492-2498.	1.1	12
6173	A Mechanistic Study of Trichoderma reesei Cel7B Catalyzed Glycosidic Bond Cleavage. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8714-8722.	1.2	19
6174	Theoretical Study on the Water-Assisted Reaction of NCO with HCHO. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6883-6892.	1.1	41
6175	Electrochemical and Density Functional Theory Investigation on High Selectivity and Sensitivity of Exfoliated Nano-Zirconium Phosphate toward Lead(II). <i>Analytical Chemistry</i> , 2013, 85, 3984-3990.	3.2	66

#	ARTICLE	IF	CITATIONS
6176	Characterization of the Thermal and Photoinduced Reactions of Photochromic Spiropyran in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2013, 117, 13561-13571.	1.2	90
6177	Alternant conjugated oligomers with tunable and narrow HOMO–LUMO gaps as sustainable nanowires. <i>RSC Advances</i> , 2013, 3, 25881.	1.7	55
6178	An Assessment of RASSCF and TDDFT Energies and Gradients on an Organic Donor–Acceptor Dye Assisted by Resonance Raman Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 543-554.	2.3	38
6179	Triple Shifts and Thioether Assistance in Rearrangements Associated with an Unusual Biomethylation of the Sterol Side Chain. <i>Journal of Organic Chemistry</i> , 2013, 78, 935-941.	1.7	12
6180	Charge and energy transfer in a bithiophene perylenediimide based donor–acceptor–donor system for use in organic photovoltaics. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11704.	1.3	20
6181	Theoretical Modeling of Deuteration-Induced Shifts of the O–O Bands in Absorption Spectra of Selected Aromatic Amines: The Role of the Double-Well Potential. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12770-12782.	1.1	6
6182	The Electronic Nature of the 1,4-β-Glycosidic Bond and Its Chemical Environment: DFT Insights into Cellulose Chemistry. <i>Chemistry - A European Journal</i> , 2013, 19, 16282-16294.	1.7	84
6183	An assessment of pure, hybrid, meta, and hybrid–meta GGA density functional theory methods for open-shell systems: The case of the nonheme iron enzyme 8-LOX. <i>Journal of Computational Chemistry</i> , 2013, 34, 141-148.	1.5	8
6184	Cis and trans-bis(tetrathiafulvalene-acetylide) platinum(II) complexes: syntheses, crystal structures, and influence of the ancillary ligands on their electronic properties. <i>Dalton Transactions</i> , 2013, 42, 383-394.	1.6	21
6185	Design of molecular switching and signaling based on proton transfer in 2-hydroxy Schiff bases: a computational study. <i>Journal of Molecular Modeling</i> , 2013, 19, 559-569.	0.8	14
6187	Charge generation/transport in organic materials. , 2013, , 219-244.		1
6188	Excited state calculations in solids by auxiliary-field quantum Monte Carlo. <i>New Journal of Physics</i> , 2013, 15, 093017.	1.2	39
6189	Electron scattering from gas phase cis-diamminedichloroplatinum(II): Quantum analysis of resonance dynamics. <i>Journal of Chemical Physics</i> , 2013, 138, 204308.	1.2	2
6190	A comparison of geometric parameters from PBE-based doubly hybrid density functionals PBE0-DH, PBE0-2, and xDH-PBE0. <i>Journal of Chemical Physics</i> , 2013, 139, 174106.	1.2	32
6191	Semilocal and hybrid meta-generalized gradient approximations based on the understanding of the kinetic-energy-density dependence. <i>Journal of Chemical Physics</i> , 2013, 138, 044113.	1.2	164
6192	Nuclear spin-spin coupling in a van der Waals-bonded system: Xenon dimer. <i>Journal of Chemical Physics</i> , 2013, 138, 104313.	1.2	13
6193	Simulation studies of the Cl ^{•-} + CH ₃ I S _N 2 nucleophilic substitution reaction: Comparison with ion imaging experiments. <i>Journal of Chemical Physics</i> , 2013, 138, 114309.	1.2	55
6194	Extreme density-driven delocalization error for a model solvated-electron system. <i>Journal of Chemical Physics</i> , 2013, 139, 184116.	1.2	93

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6195	Communication: Nuclear quadrupole moment-induced Cotton-Mouton effect in noble gas atoms. <i>Journal of Chemical Physics</i> , 2013, 139, 181102.	1.2	13
6196	Comparison between Gaussian-type orbitals and plane wave <i>ab initio</i> density functional theory modeling of layer silicates: Talc [Mg ₃ Si ₄ O ₁₀ (OH) ₂] as model system. <i>Journal of Chemical Physics</i> , 2013, 139, 204101.	1.2	44
6197	Theoretical Study of Stereoselectivity for <i>Syn</i> -Selective Cross-Aldol Reactions of Aldehydes Catalyzed by Chiral Diamine Organocatalysts. <i>Advanced Materials Research</i> , 0, 798-799, 59-62.	0.3	0
6198	Evaluation and Theoretical Study on the Anti-inflammatory Mechanism of 1-Nitro-2-phenylethane. <i>Planta Medica</i> , 2013, 79, 628-633.	0.7	18
6199	QSRR Study on GC Retention Time of Aromatic Components in Red Raspberry Wine. <i>Advanced Materials Research</i> , 2013, 781-784, 1434-1438.	0.3	1
6200	Hydrogenated <i>K</i> ₄ carbon: A new stable cubic gauche structure of carbon hydride. <i>Journal of Chemical Physics</i> , 2013, 138, 024702.	1.2	18
6201	Effect of length on the position of negative differential resistance and realization of multifunction in fused oligothiophenes based molecular device. <i>Journal of Chemical Physics</i> , 2013, 138, 074307.	1.2	12
6202	Synthesis of Liposome Reinforced with Cholesterol and Application to Transmission Electron Microscopy Observation. <i>Materials Research Society Symposia Proceedings</i> , 2013, 1498, 227-232.	0.1	1
6203	Synthesis, Spectroscopic Investigations, Quantum Chemical Studies (<i>Ab-initio</i> & <i>Tj</i> ETQqO O O rgBT /Overlock 10 prop-2-en-1-one. <i>Crystal Structure Theory and Applications</i> , 2013, 02, 167-175.	0.3	5
6204	Investigation of TiO ₂ Surface Modification with [6,6]-Phenyl-C61-butyric Acid for Titania/Polymer Hybrid Solar Cells. <i>Japanese Journal of Applied Physics</i> , 2013, 52, 112301.	0.8	4
6205	Ultrafast intersystem-crossing in platinum containing π -conjugated polymers with tunable spin-orbit coupling. <i>Scientific Reports</i> , 2013, 3, 2653.	1.6	46
6206	<i>Ab Initio</i> Calculations of Thermal Decomposition Mechanism of LiPF ₆ -Based Electrolytes for Lithium-Ion Batteries. <i>Journal of the Electrochemical Society</i> , 2013, 160, A404-A409.	1.3	40
6207	Electronic Structure Calculations in Molecules. <i>Springer Tracts in Modern Physics</i> , 2013, , 183-230.	0.1	0
6208	Phonon drag effect in nanocomposite FeSb ₂ . <i>MRS Communications</i> , 2013, 3, 31-36.	0.8	28
6209	Iminopropadienones RN=C=C=C=O and bisiminopropadienes RN=C=C=C=NR: Matrix infrared spectra and anharmonic frequency calculations. <i>Journal of Chemical Physics</i> , 2013, 139, 164314.	1.2	3
6210	Infrared and Raman Spectra of and Isotopomers: A DFT-PT2 Anharmonic Study. <i>Journal of Chemistry</i> , 2013, 2013, 1-8.	0.9	1
6211	Mechanism and Thermodynamics of Multichannel 1:1 Ammonia and Ozone Tropospheric Oxidation Reaction. <i>Progress in Reaction Kinetics and Mechanism</i> , 2013, 38, 266-282.	1.1	7
6212	Theoretical study of a reaction mechanism of tropospheric interest: CH ₃ CH ₂ F + OH. <i>Progress in Reaction Kinetics and Mechanism</i> , 2013, 38, 342-358.	1.1	0

#	ARTICLE	IF	CITATIONS
6213	Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology. Progress in Theoretical Chemistry and Physics, 2013, , .	0.2	2
6214	Second Harmonic Generation, Electrooptical Pockels Effect, and Static First-Order Hyperpolarizabilities of 2,2- β -Bithiophene Conformers: An HF, MP2, and DFT Theoretical Investigation. Advances in Physical Chemistry, 2013, 2013, 1-8.	2.0	12
6215	Understanding the Initial Decomposition Pathways of the n -Alkane/Nitroalkane Binary Mixture. Chinese Journal of Chemistry, 2013, 31, 1087-1094.	2.6	12
6216	Electronic structure and gas-phase chemistry of protonated β - and γ -quinonoid compounds: a mass spectrometry and computational study. Rapid Communications in Mass Spectrometry, 2013, 27, 816-824.	0.7	9
6217	Lowest triplet ($n, \dot{\pi}^*$) state of 2-cyclohexen-1-one: Characterization by cavity ringdown spectroscopy and quantum-chemical calculations. Journal of Chemical Physics, 2013, 139, 214311.	1.2	2
6218	Electronic states of thiophene/phenylene co-oligomers: Extreme-ultra violet excited photoelectron spectroscopy observations and density functional theory calculations. Journal of Applied Physics, 2013, 113, 083710.	1.1	14
6219	Orbital Localization, Charge Transfer, and Band Gaps in Semilocal Density-Functional Theory. Physical Review Letters, 2013, 111, 036402.	2.9	78
6220	The effect of defects and their passivation on the density of states of the 4H-silicon-carbide/silicon-dioxide interface. Journal of Applied Physics, 2013, 113, 053703.	1.1	22
6221	A DFT Study of Vibrational Spectra and Mutagenicity Predictions of Mononitrated Fluoranthenes. Polycyclic Aromatic Compounds, 2013, 33, 473-500.	1.4	4
6222	Simulation of mesogenic diruthenium tetracarboxylates: Development of a force field for coordination polymers of the MMX type. Journal of Computational Chemistry, 2013, 34, 1283-1290.	1.5	1
6223	Hybrid functionals for solids with an optimized Hartree-Fock mixing parameter. Journal of Physics Condensed Matter, 2013, 25, 435503.	0.7	74
6224	Pharmacophore modelling and electronic feature analysis of hydroxamic acid derivatives, the HIV integrase inhibitors. SAR and QSAR in Environmental Research, 2013, 24, 753-771.	1.0	8
6225	Calculation of the LSDA+ U functional using the hybrid B3LYP and HSE functionals. Physica Status Solidi (B): Basic Research, 2013, 250, 356-363.	0.7	35
6226	A benchmark study of DFT methods on the electronic properties of lanthanofullerenes: a case study of Ce@C _{2v} (9)-C ₈₂ anion. RSC Advances, 2013, 3, 26252.	1.7	2
6227	Stable Anilinyll Radicals Coordinated to Nickel: X-ray Crystal Structure and Characterization. Chemistry - A European Journal, 2013, 19, 16707-16721.	1.7	30
6228	DFT INSIGHT INTO THE UV-VIS SPECTRA AND RADICAL SCAVENGING ACTIVITY OF AURANTIO-OBTUSIN. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350024.	1.8	3
6229	Experimental and theoretical study of electronic structure of lutetium bi-phthalocyanine. Journal of Chemical Physics, 2013, 138, 234701.	1.2	15
6230	Functional derivatives of meta-generalized gradient approximation (meta-GGA) type exchange-correlation density functionals. Journal of Chemical Physics, 2013, 138, 244108.	1.2	31

#	ARTICLE	IF	CITATIONS
6231	A simplified Tamm-Dancoff density functional approach for the electronic excitation spectra of very large molecules. <i>Journal of Chemical Physics</i> , 2013, 138, 244104.	1.2	242
6232	Orbital optimized double-hybrid density functionals. <i>Journal of Chemical Physics</i> , 2013, 139, 024110.	1.2	67
6233	The reaction of formaldehyde carbonyl oxide with the methyl peroxy radical and its relevance in the chemistry of the atmosphere. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18921.	1.3	26
6234	Theoretical Study on the Mechanism of Dioxygen Evolution in Photosystem II. I. Molecular and Electronic Structures at the S ₀ , S ₁ , and S ₂ States of Oxygen-Evolving Complex. <i>Bulletin of the Chemical Society of Japan</i> , 2013, 86, 479-491.	2.0	4
6236	Pyridine-Enhanced Head-to-Tail Dimerization of Terminal Alkynes by a Rhodium-N-Heterocyclic Carbene Catalyst. <i>Chemistry - A European Journal</i> , 2013, 19, 15304-15314.	1.7	46
6237	Correlations of ion structure with multiple fragmentation pathways arising from collision-induced dissociations of selected <i>i>1</i>-hydroxycarboxylic acid anions. <i>Journal of Mass Spectrometry</i>, 2013, 48, 312-320.</i>	0.7	14
6238	Charge-transport in Organic Semiconductors: Probing High Mobility with Light. <i>Materials Research Society Symposia Proceedings</i> , 2013, 1568, 1.	0.1	0
6239	Sulfides: chemical ionization induced fragmentation studied with Proton Transfer Reaction-Mass Spectrometry and density functional calculations. <i>Journal of Mass Spectrometry</i> , 2013, 48, 367-378.	0.7	15
6240	Conformational Change from a Twisted Figure-Eight to an Open-Extended Structure in Doubly Fused 36-Å Core-Modified Octaphyrins Triggered by Protonation: Implication on Photodynamics and Aromaticity. <i>Chemistry - A European Journal</i> , 2013, 19, 17011-17020.	1.7	33
6241	Kinetics of Homolytic Substitutions by Hydrogen Atoms at Thiols and Sulfides. <i>ChemPhysChem</i> , 2013, 14, 1703-1722.	1.0	12
6242	Social Isomers of Picolines in a Small Space. <i>Chemistry - A European Journal</i> , 2013, 19, 17092-17096.	1.7	8
6243	<i>i>1</i>-Substitution Reactions of Metallabenzene: An Experimental and Computational Study. <i>Chemistry - A European Journal</i>, 2013, 19, 10982-10991.</i>	1.7	42
6244	Incorporation of Thiadiazole Derivatives as π -Spacer to Construct Efficient Metal-free Organic Dye Sensitizers for Dye-sensitized Solar Cells: A Theoretical Study. <i>Communications in Computational Chemistry</i> , 2013, 1, 152-170.	1.0	41
6245	Short Introduction to Atomic and Molecular Configuration. , 2013, , 39.		0
6246	Second-Row Transition-Metal Doping of (ZnSi) _i , i = 12, 16 Nanoclusters: Structural and Magnetic Properties. <i>Computation</i> , 2013, 1, 31-45.	1.0	5
6247	AN EXPERIMENTAL AND THEORETICAL STUDY ON IMIDAZOLIUM-BASED IONIC LIQUID PROMOTED CHLOROMETHYLATION OF AROMATIC HYDROCARBONS. <i>Journal of the Chilean Chemical Society</i> , 2013, 58, 2196-2199.	0.5	4
6248	Mapping Enzymatic Catalysis Using the Effective Fragment Molecular Orbital Method: Towards all ab initio Biochemistry. <i>PLoS ONE</i> , 2013, 8, e60602.	1.1	33
6249	Rational Design, Synthesis, and Biological Evaluation of Third Generation $\hat{\pm}$ -Noscapine Analogues as Potent Tubulin Binding Anti-Cancer Agents. <i>PLoS ONE</i> , 2013, 8, e77970.	1.1	54

#	ARTICLE	IF	CITATIONS
6250	Computational engineering of low bandgap copolymers. <i>Frontiers in Chemistry</i> , 2013, 1, 35.	1.8	59
6251	Tandem dinucleophilic cyclization of cyclohexane-1,3-diones with pyridinium salts. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 1119-1126.	1.3	3
6252	THORIA ENHANCEMENT OF NUCLEAR REACTOR SAFETY. <i>Physics International</i> , 2013, 4, 110-119.	2.0	10
6253	Interaction of Refractory Dibenzothiophenes and Polymerizable Structures. <i>International Journal of Polymer Science</i> , 2014, 2014, 1-11.	1.2	6
6254	A QUANTUM MECHANICAL STUDY OF STRUCTURAL AND ELECTRONIC DILUTION EFFECTS IN PARAMAGNETIC CHEMICAL EXCHANGE SATURATION TRANSFER AGENTS. <i>Journal of Organic and Biomolecular Simulations</i> , 2014, 1, 1-13.	1.0	1
6255	Molecular Features Related to HIV Integrase Inhibition Obtained from Structure- and Ligand-Based Approaches. <i>PLoS ONE</i> , 2014, 9, e81301.	1.1	6
6256	Prediction of Tetraoxygen Reaction Mechanism with Sulfur Atom on the Singlet Potential Energy Surface. <i>Scientific World Journal, The</i> , 2014, 2014, 1-8.	0.8	1
6257	Anharmonic Spectroscopic Investigation of Tellurophene and Its Perdeuterated Isotopomer: Application of Second-Order Perturbation Theory. <i>Journal of Quantum Chemistry</i> , 2014, 2014, 1-8.	0.6	0
6258	Hyperconjugation in Carbocations, a BLW Study with DFT approximation. <i>Frontiers in Chemistry</i> , 2014, 1, 37.	1.8	11
6259	The Dynamical Behavior of the s-Trioxane Radical Cation—A Low-Temperature EPR and Theoretical Study. <i>Molecules</i> , 2014, 19, 17305-17313.	1.7	1
6260	The Ugi four-component reaction as a concise modular synthetic tool for photo-induced electron transfer donor-anthraquinone dyads. <i>Beilstein Journal of Organic Chemistry</i> , 2014, 10, 1006-1016.	1.3	9
6261	One-pot three-component synthesis and photophysical characteristics of novel triene merocyanines. <i>Beilstein Journal of Organic Chemistry</i> , 2014, 10, 599-612.	1.3	13
6262	X-Ray, IR, NMR, UV-visible spectra and DFT analysis of 5-aryloxy-(1H)-tetrazoles, structure, conformation and tautomerism. <i>Current Chemistry Letters</i> , 2014, 3, 85-96.	0.5	2
6263	Ab initio parameterisation of the 14 band k -p Hamiltonian: Zincblende study. <i>Journal of Physics: Conference Series</i> , 2014, 526, 012004.	0.3	0
6265	Theoretical Study on Dissociation Mechanisms of Di-ethyl Berylliums and Di-t-butyl Berylliums. <i>Chinese Journal of Chemical Physics</i> , 2014, 27, 168-174.	0.6	1
6266	Hybrid Density Functional Study on Plutonium Dioxide. , 2014, , .		2
6267	Computational Study on the Structural and Electronic Properties of Multi-Nuclear Palladium and Nickel Silyl Complexes via DFT and QTAIM Approaches. <i>Molecular Crystals and Liquid Crystals</i> , 2014, 605, 89-102.	0.4	2
6268	Does NHC Directly Participate in the CO ₂ Insertion into the U ^{III} -N Bond? A Density Functional Theory Study. <i>Organometallics</i> , 2014, 33, 7007-7010.	1.1	10

#	ARTICLE	IF	CITATIONS
6269	Static second hyperpolarizability of $\hat{\Gamma}$ shaped alkaline earth metal complexes. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450039.	1.8	7
6271	Designing nonlinear optical molecule by incorporating the planar tetracoordinate unit NAI_4 - or CAI_4 - into decaborane $\text{B}_{10}\text{H}_{14}$. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450042.	1.8	0
6272	A computational study on kinetics, mechanism and thermochemistry of gas-phase reactions of 3-hydroxy-2-butanone with OH radicals. <i>Journal of Chemical Sciences</i> , 2014, 126, 1789-1801.	0.7	10
6273	Exploration for the potential precursors for zirconium carbide atomic layer deposition via comprehensive computational mechanistic study of the gas phase decomposition of neopentyl zirconium derivatives. <i>Korean Journal of Chemical Engineering</i> , 2014, 31, 2077-2080.	1.2	1
6274	Judging Density-Functional Approximations: Some Pitfalls of Statistics. <i>Topics in Current Chemistry</i> , 2014, , 81-95.	4.0	10
6275	Multiple adsorption of CO on Na-exchanged Y faujasite: a DFT investigation. <i>Molecular Simulation</i> , 2014, 40, 33-44.	0.9	15
6276	Atropisomerization in Confined Space; Cucurbiturils as Tools to Determine the Torsional Barrier of Substituted Biphenyls. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 105-110.	1.2	8
6277	The dynamics of interconverting D- and E-forms of the HIV-1 integrase N-terminal domain. <i>European Biophysics Journal</i> , 2014, 43, 485-498.	1.2	5
6278	Assessment of theoretical procedures for a diverse set of isomerization reactions involving double-bond migration in conjugated dienes. <i>Chemical Physics</i> , 2014, 441, 166-177.	0.9	49
6279	Liquid-Liquid Extraction of Acids and Water by a Malonamide: I-Anion Specific Effects on the Polar Core Microstructure of the Aggregated Malonamide. <i>Solvent Extraction and Ion Exchange</i> , 2014, 32, 601-619.	0.8	35
6280	Gas-phase reaction of ClO^{\bullet} with $\text{CH}_n\text{Cl}_{4-n}$ ($n = 0, 1, 2, 3$) and CX_3H ($X = \text{F}, \text{Cl}$ and Br): Substituent effect from a comparative study. <i>Canadian Journal of Chemistry</i> , 2014, 92, 868-875.	0.6	1
6281	An experimental and theoretical study of the resonant Auger spectrum of the ethene molecule. <i>New Journal of Physics</i> , 2014, 16, 073022.	1.2	1
6282	Band alignment and optical absorption in Ga(Sb)N alloys. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 055013.	0.7	14
6283	The structure of protonated 3-pyridyl-substituted 5-amino-1H-1,2,4-triazoles: an experimental and theoretical study. <i>Russian Chemical Bulletin</i> , 2014, 63, 2591-2598.	0.4	1
6284	Determination of acidic dissociation constants of glutamine and isoleucine in water using ab initio methods. <i>Turkish Journal of Biochemistry</i> , 0, , .	0.3	1
6285	Glycosaminoglycan Monosaccharide Blocks Analysis by Quantum Mechanics, Molecular Dynamics, and Nuclear Magnetic Resonance. <i>BioMed Research International</i> , 2014, 2014, 1-11.	0.9	13
6286	Highly regioselective hydride transfer, oxidative dehydrogenation, and hydrogen-atom abstraction in the thermal gas-phase chemistry of $[\text{Zn}(\text{OH})]^{++}/\text{C}_3\text{H}_8$. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26617-26623.	1.3	11
6287	A first-principles polarized Raman method for determining whether a uniform region of a sample is crystalline or isotropic. <i>Journal of Chemical Physics</i> , 2014, 141, 224702.	1.2	1

#	ARTICLE	IF	CITATIONS
6288	Nuclear spin circular dichroism. <i>Journal of Chemical Physics</i> , 2014, 140, 134103.	1.2	20
6289	Electronic Structures, DNA-binding, SAR, and Spectral Properties of Ruthenium Methylimidazole Complexes [Ru(Melm) ₄ L] ₂ ⁺ (L=iip, tip, 2ntz). <i>Chinese Journal of Chemical Physics</i> , 2014, 27, 159-167.	0.6	3
6290	Structural, vibrational, elastic and topological properties of PaN under pressure. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 035403.	0.7	3
6291	Experimental and theoretical studies of 2- <i>amino</i> thiazole as an inhibitor for carbon steel corrosion in hydrochloric acid. <i>Materials and Corrosion - Werkstoffe Und Korrosion</i> , 2014, 65, 1194-1201.	0.8	21
6292	Slow Reactant-Water Exchange and High Catalytic Performance of Water-Tolerant Lewis Acids. <i>Chemistry - A European Journal</i> , 2014, 20, 8068-8075.	1.7	33
6293	Energetics of heterometal substitution in \hat{A} -Keggin [MO ₄ Al ₁₂ (OH) ₂₄ (OH ₂) ₁₂] _{6/7/8+} ions. <i>American Mineralogist</i> , 2014, 99, 2337-2343.	0.9	7
6294	Analysis of nonlinear optical properties in donor-acceptor materials. <i>Journal of Chemical Physics</i> , 2014, 140, 184308.	1.2	32
6295	A self-interaction-free local hybrid functional: Accurate binding energies vis-à-vis accurate ionization potentials from Kohn-Sham eigenvalues. <i>Journal of Chemical Physics</i> , 2014, 140, 18A510.	1.2	66
6296	Oxorhenium(V) Complexes with Phenolate-Oxazoline Ligands: Influence of the Isomeric Form on the O-Atom-Transfer Reactivity. <i>Inorganic Chemistry</i> , 2014, 53, 12918-12928.	1.9	28
6297	Density functional investigation of intermolecular effects on ¹³ C NMR chemical-shielding tensors modeled with molecular clusters. <i>Journal of Chemical Physics</i> , 2014, 141, 164121.	1.2	53
6298	Point defects as a test ground for the local density approximation +U theory: Mn, Fe, and VGa in GaN. <i>Journal of Chemical Physics</i> , 2014, 141, 114703.	1.2	14
6299	A computational study of potential molecular switches that exploit Baird's rule on excited-state aromaticity and antiaromaticity. <i>Faraday Discussions</i> , 2014, 174, 105-124.	1.6	22
6300	Describing long-range charge-separation processes with subsystem density-functional theory. <i>Journal of Chemical Physics</i> , 2014, 140, 164103.	1.2	39
6301	Smallest fullerene-like silicon cage stabilized by a V ₂ unit. <i>Journal of Chemical Physics</i> , 2014, 140, 024308.	1.2	47
6302	Structural, electronic, and optical properties of GaInO ₃ : A hybrid density functional study. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	33
6303	TDDFT Assessment of Functionals for Optical \hat{O} Transitions in Small Radicals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11033-11046.	1.1	15
6304	Access to Polycyclic Derivatives by Triflate-Catalyzed Intramolecular Hydroarylation. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 7458-7468.	1.2	23
6305	Effect of Extended Conjugation on the Optoelectronic Properties of Benzo[1,2-d:4,5-d']bioxazole Polymers. <i>Australian Journal of Chemistry</i> , 2014, 67, 711.	0.5	10

#	ARTICLE	IF	CITATIONS
6306	Practical auxiliary basis implementation of Rung 3.5 functionals. <i>Journal of Chemical Physics</i> , 2014, 141, 034103.	1.2	23
6307	A DFT-based model for calculating solvolytic reactivity. The nucleofugality of aliphatic carboxylates in terms of N_{f} parameters. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 5698.	1.5	17
6308	Spin-State-Dependent Properties of an Iron(III) Hydrogenase Mimic. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 3587-3599.	1.0	12
6309	Solvolysis Mechanisms of RNA Phosphodiester Analogues Promoted by Mononuclear Zinc(II) Complexes: Mechanistic Determination upon Solvent Medium and Ligand Effects. <i>Inorganic Chemistry</i> , 2014, 53, 11903-11912.	1.9	10
6310	Theoretical investigation of atomic oxygen erosion mechanisms of 1,3-didecyl cyclopentane, 1,3-dioctyldecyl cyclopentane and alkylated cyclopentane. <i>RSC Advances</i> , 2014, 4, 50486-50493.	1.7	4
6311	Reductive Functionalization of a Rhodium(III)–Methyl Bond in Acidic Media: Key Step in the Electrophilic Functionalization of Methane. <i>Organometallics</i> , 2014, 33, 6504-6510.	1.1	22
6312	Electrosynthesis of Poly(alanine)-Like Peptides in Concentrated Alanine Based Electrolytes, Characterization Coupled to DFT Study and Application to pH Proton Receptor. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25041-25050.	1.5	6
6313	Tuning of the HOMO–LUMO gap of donor-substituted symmetrical and unsymmetrical benzothiadiazoles. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 5448.	1.5	63
6314	Self-consistent linear response for the spin-orbit interaction related properties. <i>Physical Review B</i> , 2014, 90, .	1.1	22
6315	Mechanistic photodecarboxylation of pyruvic acid: Excited-state proton transfer and three-state intersection. <i>Journal of Chemical Physics</i> , 2014, 141, 154311.	1.2	44
6316	Tricks of Light on Helices: Transformation of Helical Polymers by Photoirradiation. <i>Chemical Record</i> , 2014, 14, 369-385.	2.9	41
6317	Nuclear quadrupole moment-induced Cotton-Mouton effect in molecules. <i>Journal of Chemical Physics</i> , 2014, 140, 024103.	1.2	11
6318	Thermal decomposition of 1,3,3-trinitroazetidine (TNAZ): A density functional theory and ab initio study. <i>Journal of Chemical Physics</i> , 2014, 140, 154306.	1.2	3
6319	Quantum mechanical modeling of hydrolysis and H ₂ O-exchange in Mg-, Ca-, and Ni-silicate clusters: Implications for dissolution mechanisms of olivine minerals. <i>American Mineralogist</i> , 2014, 99, 2303-2312.	0.9	12
6320	Kohn-Sham potentials in exact density-functional theory at noninteger electron numbers. <i>Physical Review A</i> , 2014, 90, .	1.0	42
6321	The one-electron oxidation of a dithiolate molecule: The importance of chemical intuition. <i>Journal of Chemical Physics</i> , 2014, 140, 18A519.	1.2	8
6322	Toward a Unified Model of Passive Drug Permeation II: The Physicochemical Determinants of Unbound Tissue Distribution with Applications to the Design of Hepatoselective Glucokinase Activators. <i>Drug Metabolism and Disposition</i> , 2014, 42, 1599-1610.	1.7	19
6323	Assessment of density functional theory based $\hat{\rho}^{\text{SCF}}$ (self-consistent field) and linear response methods for longest wavelength excited states of extended π -conjugated molecular systems. <i>Journal of Chemical Physics</i> , 2014, 141, 024112.	1.2	39

#	ARTICLE	IF	CITATIONS
6324	Coupledâ€cluster reaction barriers of : An application of the coupledâ€cluster//Kohnâ€Sham density functional theory model chemistry. <i>Journal of Computational Chemistry</i> , 2014, 35, 507-517.	1.5	20
6325	A Theoretical and Experimental Study of the Effects of Silyl Substituents in Enantioselective Reactions Catalyzed by Diphenylprolinol Silyl Ether. <i>Chemistry - A European Journal</i> , 2014, 20, 17077-17088.	1.7	54
6326	A little spin on the side: solvent and temperature dependent paramagnetism in [RuII(bpy)2(phendione)]2+. <i>Dalton Transactions</i> , 2014, 43, 17729-17739.	1.6	7
6327	Combined hybrid functional and DFT+ <i>U</i> calculations for metal chalcogenides. <i>Journal of Chemical Physics</i> , 2014, 141, 044106.	1.2	37
6328	Theoretical prediction of nuclear magnetic shieldings and indirect spin-spin coupling constants in 1,1-, cis-, and trans-1,2-difluoroethylenes. <i>Journal of Chemical Physics</i> , 2014, 140, 144303.	1.2	21
6329	Hybrid density functional theory study of Cu(In1âˆxGax)Se2 band structure for solar cell application. <i>AIP Advances</i> , 2014, 4, .	0.6	19
6330	Halogen Bonding from Dispersion-Corrected Density-Functional Theory: The Role of Delocalization Error. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5436-5447.	2.3	100
6331	Solventâ€induced conformational flexibility of a bicyclic proline analogue: Octahydroindoleâ€2â€carboxylic acid. <i>Biopolymers</i> , 2014, 102, 176-190.	1.2	1
6332	Robust and efficient variational fitting of Fock exchange. <i>Journal of Chemical Physics</i> , 2014, 141, 124114.	1.2	58
6333	Oddâ€hydrogen: An account on electronic structure, kinetics, and role of water in mediating reactions with atmospheric ozone. Just a catalyst or far beyond?. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1327-1349.	1.0	21
6334	Gated Electron Sharing Within Dynamic Naphthalene Diimideâ€Based Oligorotaxanes. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 4442-4449.	7.2	57
6335	A mechanistic and experimental study on the diethyl ether oxidation. <i>Process Safety Progress</i> , 2014, 33, 64-69.	0.4	16
6336	Effect of the Metal Ion on the anti <i>T. cruzi</i> Activity and Mechanism of Action of 5â€Nitrofurylâ€Containing Thiosemicarbazone Metal Complexes. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 4677-4689.	1.0	26
6337	Pyridineâ€ <i>N</i> -oxide 2â€Carboxylic Acid: An Acceptor Group for Organic Sensitizers with Enhanced Anchoring Stability in Dyeâ€Sensitized Solar Cells. <i>Asian Journal of Organic Chemistry</i> , 2014, 3, 140-152.	1.3	18
6338	A computational perspective on the kinetics and thermochemistry of the gas phase reactions of 1, 1-dichlorodimethylether (DCDME) with OH radical at 298â€K. <i>Molecular Physics</i> , 2014, 112, 1512-1519.	0.8	11
6339	Importance of high-angular-momentum channels in pseudopotentials for quantum Monte Carlo. <i>Physical Review B</i> , 2014, 90, .	1.1	8
6340	Density Functional Theory Beyond the Generalized Gradient Approximation for Surface Chemistry. <i>Topics in Current Chemistry</i> , 2014, , 25-51.	4.0	9
6341	Theoretical investigation of molecular and electronic structure changes of the molecular magnet Mn₁₂ cluster upon superâ€reduction. <i>Physica Status Solidi - Rapid Research Letters</i> , 2014, 8, 517-521.	1.2	3

#	ARTICLE	IF	CITATIONS
6342	Approximating the exchange energy through the nonempirical exchange-factor approach. <i>Physical Review A</i> , 2014, 90, .	1.0	16
6343	Reaction of Hydrazine with a Chlorine-Terminated Si(111) Surface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27998-28006.	1.5	22
6344	Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation. <i>Journal of Chemical Physics</i> , 2014, 141, 024114.	1.2	42
6346	Nuclear-spin-induced Cotton-Mouton Effect in a Strong External Magnetic Field. <i>ChemPhysChem</i> , 2014, 15, 2337-2350.	1.0	10
6347	A designed bithiopheneimide-based conjugated polymer for organic photovoltaic with ultrafast charge transfer at donor/PC71BM interface: theoretical study and characterization. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 25799-25808.	1.3	51
6348	Communication: An N-body solution to the problem of Fock exchange. <i>Journal of Chemical Physics</i> , 2014, 140, 111101.	1.2	2
6349	Vibronic coupling in asymmetric bichromophores: Theory and application to diphenylmethane-d5. <i>Journal of Chemical Physics</i> , 2014, 141, 134119.	1.2	9
6350	A material design of a new high-performance ferroelectric. I. SrTiO ₂ C perovskite. <i>Molecular Physics</i> , 2014, 112, 533-538.	0.8	5
6351	The DFT+U method and its application to the adsorption of CO on platinum model clusters. <i>Journal of Chemical Physics</i> , 2014, 140, 174709.	1.2	10
6353	Theoretical study of hyperfine interactions and optically detected magnetic resonance spectra by simulation of the C ₂₉₁ [NV] ⁻ H ₁₇₂ diamond cluster hosting nitrogen-vacancy center. <i>New Journal of Physics</i> , 2014, 16, 083014.	1.2	23
6354	Computational evaluation of unsaturated carbonitriles as neutral receptor model for beryllium(II) recognition. <i>Journal of Molecular Modeling</i> , 2014, 20, 2533.	0.8	0
6355	Arene-fused 1,2-oxazole N-oxides and derivatives. The impact of the N=O dipole and substitution on their aromatic character and reactivity profile. Can it be a useful structure in synthesis? A theoretical insight. <i>Structural Chemistry</i> , 2014, 25, 1837-1846.	1.0	4
6356	Trapping in water – an important prerequisite for complex reactivity in astrophysical ices: the case of acetone (CH ₃) ₂ C=O and ammonia NH ₃ . <i>Monthly Notices of the Royal Astronomical Society</i> , 2014, 443, 2991-3000.	1.6	21
6357	Towards a Mechanism Underlying the Stability of the Tetragonal CuO Phase: Comparison with NiO and CoO by Hybrid Density Functional Calculation. <i>Chinese Physics Letters</i> , 2014, 31, 027402.	1.3	6
6358	Direct computation of parameters for accurate polarizable force fields. <i>Journal of Chemical Physics</i> , 2014, 141, 194114.	1.2	28
6359	Theoretical study on the gas phase reaction of allyl chloride with hydroxyl radical. <i>Journal of Chemical Physics</i> , 2014, 140, 084309.	1.2	5
6360	Arsenic Adsorption onto Minerals: Connecting Experimental Observations with Density Functional Theory Calculations. <i>Minerals (Basel, Switzerland)</i> , 2014, 4, 208-240.	0.8	58
6361	Armed-Disarmed Concept in the Synthesis of Glycosidic Bond. , 2014, , 117-179.		0

#	ARTICLE	IF	CITATIONS
6362	Living Supramolecular Compounds: Influence of Multiple Hydrogen Bond Connection on Molecular Configuration of Monophosphate or Pyrophosphate Thiamine with Anions or Coordination Anions. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2014, 640, 2981-2990.	0.6	2
6363	The Ring and Exchange-Ring Approximations Based on Kohn-Sham Reference States. <i>Topics in Current Chemistry</i> , 2014, , 97-144.	4.0	3
6364	Aprotic Electrolytes in Li-Air Batteries. <i>Modern Aspects of Electrochemistry</i> , 2014, , 445-466.	0.2	0
6365	8th Congress on Electronic Structure: Principles and Applications (ESPA 2012). <i>Highlights in Theoretical Chemistry</i> , 2014, , .	0.0	0
6366	Cascade cyclization of 1-(2-yl-3-phenylprop-2-enyl)-6-oxo-1,6-dihydropyridine-2-carbonitrile radical: Mechanistic insights from DFT study. <i>Computational and Theoretical Chemistry</i> , 2014, 1044, 1-9.	1.1	6
6367	Progress on New Approaches to Old Ideas: Orbital-Free Density Functionals. <i>Letters in Mathematical Physics</i> , 2014, , 113-134.	0.4	30
6368	The Potential Utility of Predicted One Bond Carbon-Proton Coupling Constants in the Structure Elucidation of Small Organic Molecules by NMR Spectroscopy. <i>PLoS ONE</i> , 2014, 9, e111576.	1.1	12
6369	Computational Redox Potential Predictions: Applications to Inorganic and Organic Aqueous Complexes, and Complexes Adsorbed to Mineral Surfaces. <i>Minerals (Basel, Switzerland)</i> , 2014, 4, 345-387.	0.8	56
6370	Unraveling polar Diels-Alder reactions with conceptual DFT analysis and the distortion/interaction model. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 187-199.	1.5	31
6371	Experimental and quantum chemical studies of the effect of poly ethylene glycol as corrosion inhibitors of aluminum surface. <i>Journal of Industrial and Engineering Chemistry</i> , 2014, 20, 796-808.	2.9	93
6372	Structure and properties of cerium oxides in bulk and nanoparticulate forms. <i>Journal of Alloys and Compounds</i> , 2014, 584, 199-208.	2.8	79
6373	The polymerisation of oligo(ethylene glycol methyl ether) methacrylate from a multifunctional poly(ethylene imine) derived amide: a stabiliser for the synthesis and dispersion of magnetite nanoparticles. <i>Polymer Chemistry</i> , 2014, 5, 524-534.	1.9	12
6374	Frontiers of stable isotope geoscience. <i>Chemical Geology</i> , 2014, 372, 119-143.	1.4	99
6375	Theoretical study of the absorption and emission spectra of the anionic p-coumaric methyl ester in gas phase and in solution. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 287-294.	1.1	6
6376	Charge distribution of poly (p-phenylene benzobisoxazole) investigated by quantum chemical simulation. <i>Computational and Theoretical Chemistry</i> , 2014, 1042, 1-7.	1.1	4
6377	Mechanism and origins of enantioselectivity for [BMIM]Cl ionic liquids and ZnCl ₂ co-catalyzed coupling reaction of CO ₂ with epoxides. <i>Journal of Molecular Catalysis A</i> , 2014, 385, 133-140.	4.8	34
6378	Mechanisms of chromate adsorption on hematite. <i>Geochimica Et Cosmochimica Acta</i> , 2014, 138, 146-157.	1.6	91
6379	A computational approach to the electronic, optical and acid-base properties of Ru(II) dyes for photoelectrochemical solar cells applications. <i>Polyhedron</i> , 2014, 82, 88-103.	1.0	3

#	ARTICLE	IF	CITATIONS
6380	On the ferryl catalyst: Electronic structure and optimized ab initio geometry. <i>Chemical Physics Letters</i> , 2014, 595-596, 175-179.	1.2	5
6381	5-Phenyl-iminostilbene based organic dyes for efficient dye-sensitized solar cells. <i>Tetrahedron</i> , 2014, 70, 6241-6248.	1.0	1
6382	turboTDDFT 2.0's Hybrid functionals and new algorithms within time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , 2014, 185, 2080-2089.	3.0	55
6383	Theoretical study of the reaction mechanism of a series of 4-hydroxycoumarins against the DPPH radical. <i>Chemical Physics Letters</i> , 2014, 601, 116-123.	1.2	7
6384	Theoretical design of thiazolothiazole-based organic dyes with different electron donors for dye-sensitized solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 232-238.	2.0	61
6385	Theoretical investigation of phenothiazine's triphenylamine-based organic dyes with different π spacers for dye-sensitized solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 123, 282-289.	2.0	25
6386	In silico design of a tunable molecular spin filter using chromium's carbon's chromium chains. <i>Chemical Physics</i> , 2014, 428, 34-42.	0.9	5
6387	DFT calculations, spectroscopic, thermal analysis and biological activity of Sm(III) and Tb(III) complexes with 2-aminobenzoic and 2-amino-5-chloro-benzoic acids. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 131, 388-397.	2.0	19
6388	Periodic density functional theory study on the interaction mode and mechanism of typical additives with TiO ₂ substrates for dye-sensitized solar cell applications. <i>Journal of Power Sources</i> , 2014, 246, 10-18.	4.0	16
6389	Theoretical investigation of inhibition of the corrosion of A106 steel in NaCl solution by di-n-butyl bis(thiophene-2-carboxylato-O,O's tin(IV). <i>Research on Chemical Intermediates</i> , 2014, 40, 569-586.	1.3	12
6390	Theoretical studies of the reaction of hydroxyl radical with cyclopentane (C ₅ H ₁₀). <i>Molecular Physics</i> , 2014, 112, 963-971.	0.8	9
6391	Redox and photoisomerisation switching the second-order nonlinear optical properties of a tetrathiafulvalene derivative across ten stable states: a DFT study. <i>Molecular Physics</i> , 2014, 112, 199-205.	0.8	8
6392	Exploring the vibrational fingerprint of the electronic excitation energy via molecular dynamics. <i>Journal of Chemical Physics</i> , 2014, 140, 134105.	1.2	5
6393	Mechanism of Asymmetric Hydrogenation of \hat{I}^2 -Dehydroamino Acids Catalyzed by Rhodium Complexes: Large-Scale Experimental and Computational Study. <i>ACS Catalysis</i> , 2014, 4, 203-219.	5.5	43
6394	Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2014, 372, 20120476.	1.6	599
6395	First-principles calculations for point defects in solids. <i>Reviews of Modern Physics</i> , 2014, 86, 253-305.	16.4	1,967
6396	Efficiency enhancement of black dye-sensitized solar cells by newly synthesized D's I's A coadsorbents: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9499-9508.	1.3	13
6397	A combined experimental and TD-DFT investigation of three disperse azo dyes having the nitroterephthalate skeleton. <i>Dyes and Pigments</i> , 2014, 103, 25-33.	2.0	32

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6398	Charge Storage in Decyl- and 3,6,9-Trioxadecyl-Substituted Poly(dithieno[3,2- <i>b</i> :2,3- <i>d</i>]pyrrole) Electrodes. <i>Macromolecules</i> , 2014, 47, 79-88.	2.2	26
6399	Equimolar Carbon Absorption by Potassium Phthalimide and In Situ Catalytic Conversion Under Mild Conditions. <i>ChemSusChem</i> , 2014, 7, 1484-1489.	3.6	45
6400	Effects of Electrodes and Nitrogen-Atom Locations on Electron Transport in C59N Molecular Junctions: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 617-626.	1.5	9
6401	Understanding the Reactivity Difference of Isocyanate and Isothiocyanate toward a Ruthenium Silylene Hydride Complex. <i>Organometallics</i> , 2014, 33, 892-897.	1.1	28
6402	Bonds, bands, and band gaps in tetrahedrally bonded ternary compounds: The role of group V lone pairs. <i>Journal of Physics and Chemistry of Solids</i> , 2014, 75, 477-485.	1.9	27
6403	Density functional theory investigation of the electronic structure and thermoelectric properties of layered MoS ₂ , MoSe ₂ and their mixed-layer compound. <i>Journal of Solid State Chemistry</i> , 2014, 211, 113-119.	1.4	40
6404	Diverse in vitro and in vivo anti-inflammatory effects of trichlorido-gold(III) complexes with N ⁶ -benzyladenine derivatives. <i>Journal of Inorganic Biochemistry</i> , 2014, 134, 92-99.	1.5	12
6405	Impact of local compressive stress on the optical transitions of single organic dye molecules. <i>Nature Nanotechnology</i> , 2014, 9, 182-186.	15.6	22
6406	Cytotoxic effects of dillapiole on MDA-MB-231 cells involve the induction of apoptosis through the mitochondrial pathway by inducing an oxidative stress while altering the cytoskeleton network. <i>Biochimie</i> , 2014, 99, 195-207.	1.3	25
6407	Dissecting molecular descriptors into atomic contributions in density functional reactivity theory. <i>Journal of Chemical Physics</i> , 2014, 140, 024109.	1.2	34
6408	Phosphate Monoester Hydrolysis by Trinuclear Alkaline Phosphatase; DFT Study of Transition States and Reaction Mechanism. <i>ChemPhysChem</i> , 2014, 15, 2321-2330.	1.0	27
6409	Prediction of hydration free energies for the SAMPL4 data set with the AMOEBA polarizable force field. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 235-244.	1.3	16
6410	Molecular properties of the PCO radical: heat of formation and the isomerization pathways. <i>Journal of Molecular Modeling</i> , 2014, 20, 2074.	0.8	14
6411	Simulating Cl K-edge X-ray absorption spectroscopy in MCl ₆ 2 ⁺ (M = U, Np, Pu) complexes and UOCl ₅ ⁺ using time-dependent density functional theory. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	11
6412	Collision-Induced Dissociation of Diazirine-Labeled Peptide Ions. Evidence for Brønsted-Acid Assisted Elimination of Nitrogen. <i>Journal of the American Society for Mass Spectrometry</i> , 2014, 25, 778-789.	1.2	18
6413	Group VB transition metal oxide clusters M ₄ O _n (M = Nb, Ta; n = 11): structural evolution and chemical bonding. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	3
6414	Structures and binding energies of the (dibenzoylmethanato)boron difluoride complexes with aromatic hydrocarbons in the ground and excited states. Density functional theory calculations. <i>High Energy Chemistry</i> , 2014, 48, 24-29.	0.2	12
6415	A DFT study on structural and electronic properties of Mn substituted CdO nanoclusters. <i>European Physical Journal D</i> , 2014, 68, 1.	0.6	3

#	ARTICLE	IF	CITATIONS
6416	Theoretical study on the gas phase reaction of acrylonitrile with atomic hydrogen. <i>Structural Chemistry</i> , 2014, 25, 1217-1227.	1.0	4
6417	Assessment of various density functionals for intermolecular Na ⁺ Sn interactions: The test case of trimethyltin cyanide dimer. <i>Computational and Theoretical Chemistry</i> , 2014, 1036, 31-43.	1.1	7
6418	Polyhydroxylated macrolide isolated from the endophytic fungus <i>Pestalotiopsis mangiferae</i> . <i>Tetrahedron Letters</i> , 2014, 55, 2642-2645.	0.7	19
6419	A combined theoretical and experimental investigation on the solvatochromism of ESIPT3-(1,3-benzothiazol-2-yl)-2-hydroxynaphthalene-1-carbaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 127, 16-24.	2.0	9
6420	Helical Carbon Segment in Carbon-Boron-Nitride Heteronanotubes: Structure and Nonlinear Optical Properties. <i>ChemPlusChem</i> , 2014, 79, 732-736.	1.3	16
6421	Theoretical Considerations and Computational Tools. <i>Advances in Experimental Medicine and Biology</i> , 2014, 794, 69-93.	0.8	0
6422	Quantum mechanical study of solvent effects in a prototype S _N 2 reaction in solution: Cl ⁻ attack on CH ₃ Cl. <i>Journal of Chemical Physics</i> , 2014, 140, 054109.	1.2	16
6423	Toward an Optomechanical Control of Photoswitches by Tuning Their Spectroscopical Properties: Structural and Dynamical Insights into Azobenzene. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 312-323.	2.3	24
6424	DFT studies on the tetranuclear cubane complex [Ni ₄ (ampd) ₄ (Cl ₄)]·MeCN. <i>Journal of Structural Chemistry</i> , 2014, 55, 30-37.	0.3	4
6425	Theoretical study for the CH ₃ C(O)(CH ₂) ₂ OH+OH reaction. <i>Structural Chemistry</i> , 2014, 25, 607-615.	1.0	15
6426	Structural characteristics of coal functional groups using quantum chemistry for quantification of infrared spectra. <i>Fuel Processing Technology</i> , 2014, 118, 287-295.	3.7	131
6427	Synthesis of novel styryl derivatives from 4-chloro-2-(morpholin-4-yl)-1,3-thiazole-5-carbaldehyde, study of their photophysical properties and TD-DFT computations. <i>Journal of Luminescence</i> , 2014, 150, 8-18.	1.5	9
6428	Palladium-Catalyzed <i>Meta</i> -Selective C-H Bond Activation with a Nitrile-Containing Template: Computational Study on Mechanism and Origins of Selectivity. <i>Journal of the American Chemical Society</i> , 2014, 136, 344-355.	6.6	317
6429	Theoretical investigation of new thiazolothiazole-based D-π-A organic dyes for efficient dye-sensitized solar cell. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 124, 646-654.	2.0	79
6430	New semiconducting naphthalene bisimides N-substituted with alkoxyphenyl groups: spectroscopic, electrochemical, structural and electrical properties. <i>RSC Advances</i> , 2014, 4, 14089-14100.	1.7	12
6431	Pd-catalyzed bicyclization of 2-alkynylhalobenzenes and propargylic alcohols for the formation of indeno[1,2]furans: a DFT study. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 237-244.	0.9	3
6432	Organic dyes with imidazole derivatives as auxiliary donors for dye-sensitized solar cells: Experimental and theoretical investigation. <i>Dyes and Pigments</i> , 2014, 104, 48-56.	2.0	31
6433	Introducing constricted variational density functional theory in its relaxed self-consistent formulation (RSCF-CV-DFT) as an alternative to adiabatic time dependent density functional theory for studies of charge transfer transitions. <i>Journal of Chemical Physics</i> , 2014, 140, 18A502.	1.2	26

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6434	Sulfonyl Acetylenes as Alkynylating Reagents Under Radical or Anionic Conditions. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 1577-1588.	1.2	35
6435	TDDFT study of UV-vis spectra of permethrin, cypermethrin and their beta-cyclodextrin inclusion complexes: A comparison of dispersion correction DFT (DFT-D3) and DFT. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 461-467.	2.0	18
6436	Theoretical Study of Reductive Functionalization of Methyl Ligands of Group 9 Complexes Supported by Two Bipyridyl Ligands: A Key Step in Catalytic Hydrocarbon Functionalization. <i>Organometallics</i> , 2014, 33, 1936-1944.	1.1	15
6437	Quantitative structure-activity relationship model for amino acids as corrosion inhibitors based on the support vector machine and molecular design. <i>Corrosion Science</i> , 2014, 83, 261-271.	3.0	132
6438	Nickel(I) Monomers and Dimers with Cyclopentadienyl and Indenyl Ligands. <i>Chemistry - A European Journal</i> , 2014, 20, 5327-5337.	1.7	65
6439	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. <i>Topics in Current Chemistry</i> , 2014, , 1-23.	4.0	17
6440	Calculation of metallic and insulating phases of V ₂ O ₃ by hybrid density functionals. <i>Journal of Chemical Physics</i> , 2014, 140, 054702.	1.2	24
6441	Inclusion complexes of cypermethrin and permethrin with monochlorotriazinyl-beta-cyclodextrin: A combined spectroscopy, TG/DSC and DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 117, 576-586.	2.0	22
6442	Iridium-Catalyzed Hydrogen Production from Hydrosilanes and Water. <i>ChemCatChem</i> , 2014, 6, 1691-1697.	1.8	41
6443	Theoretical and Experimental Study on the Inhibition of Diethyl Ether Oxidation. <i>Energy & Fuels</i> , 2014, 28, 2821-2829.	2.5	7
6444	Theoretical study on the degradation reaction mechanism of elimination hydrogen fluoride from perfluoropropionic acid. <i>Computational and Theoretical Chemistry</i> , 2014, 1029, 33-40.	1.1	7
6445	Isomerism of Cycloserine and Its Protonated Form. <i>ChemPlusChem</i> , 2014, 79, 584-591.	1.3	5
6446	Short-range exact exchange effects in ultra-narrow zigzag silicon carbide nanoribbons. <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 423-434.	0.7	10
6447	DFT investigation of structural and vibrational properties of type B and mixed A-B carbonated hydroxylapatite. <i>American Mineralogist</i> , 2014, 99, 117-127.	0.9	35
6448	Benchmarking Hydrogen and Carbon NMR Chemical Shifts at HF, DFT, and MP2 Levels. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 572-578.	2.3	152
6449	Evaluation of antibacterial properties of novel phthalocyanines against <i>Escherichia coli</i> - Comparison of analytical methods. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2014, 138, 230-239.	1.7	31
6450	A rational design for the selective detection of dopamine using conducting polymers. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7850-7861.	1.3	43
6451	Alkoxy-Functionalized Thienyl-Vinylene Polymers for Field-Effect Transistors and All-Polymer Solar Cells. <i>Advanced Functional Materials</i> , 2014, 24, 2782-2793.	7.8	83

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6452	Computational investigations on the catalytic mechanism of maleate isomerase: the role of the active site cysteine residues. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12462-12474.	1.3	6
6453	Construction of a parameter-free doubly hybrid density functional from adiabatic connection. <i>Journal of Chemical Physics</i> , 2014, 140, 18A512.	1.2	57
6454	Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1934-1952.	2.3	128
6455	Characterization of two new (Aâ€“í€)2â€“Dâ€“A type dyes with different central D unit and their application for dye sensitized solar cells. <i>Organic Electronics</i> , 2014, 15, 1780-1790.	1.4	13
6456	Molecular Structure of 3-Amino[1,2,4]Triazolo-[4,3-A]Pyrimidin-5-One in Various Tautomeric Forms: Investigation by DFT and QTAIM Methods. <i>Chemistry of Heterocyclic Compounds</i> , 2014, 50, 319-326.	0.6	12
6457	Electropolymerization mechanisms of hydroxyphenylacetic acid isomers. <i>Journal of Molecular Structure</i> , 2014, 1072, 298-306.	1.8	15
6458	Charge-Delocalized η^2 -C</i>, <i>N</i>-NHC-Amine Complexes of Rhodium, Iridium, and Ruthenium. <i>Organometallics</i> , 2014, 33, 2853-2861.	1.1	7
6459	Photophysical properties of Schiffâ€™s bases from 3-(1,3-benzothiazol-2-yl)-2-hydroxy naphthalene-1-carbaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 678-686.	2.0	12
6460	Mechanism of Carbon Monoxide Induced Nâ€“N Bond Cleavage of Nitrous Oxide Mediated by Molybdenum Complexes: A DFT Study. <i>Organometallics</i> , 2014, 33, 1553-1562.	1.1	7
6461	Theoretical Study for the Reactions of (Silyl)(silylene)tungsten and -molybdenum Complexes with Ethylene Sulfide. <i>Organometallics</i> , 2014, 33, 2704-2712.	1.1	5
6462	Direct Probing of Photoinduced Electron Transfer in a Self-Assembled Biomimetic [2Fe2S]-Hydrogenase Complex Using Ultrafast Vibrational Spectroscopy. <i>Inorganic Chemistry</i> , 2014, 53, 5373-5383.	1.9	43
6463	Functionalization of Complexed N_{2O} in Bis(pentamethylcyclopentadienyl) Systems of Zirconium and Titanium. <i>Organometallics</i> , 2014, 33, 2760-2769.	1.1	18
6464	Band offsets of lattice-matched semiconductor heterojunctions through hybrid functionals andGOWO. <i>Physical Review B</i> , 2014, 89, .	1.1	100
6465	First principle investigations to enhance the charge transfer properties by bridge elongation. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450013.	1.8	14
6466	The effect of noble metals in Si nanocrystals. <i>Chemical Physics Letters</i> , 2014, 605-606, 38-43.	1.2	5
6467	Inclusion of cybotactic effect in the theoretical modeling of absorption spectra of liquid-state systems with perturbed matrix method and molecular dynamics simulations: the UVâ€“Vis absorption spectrum of para-nitroaniline as a case study. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	5
6468	Vibrational and Electronic Spectra of Silole: A Theoretical PT2-DFT Anharmonic and TD-DFT Study. <i>Journal of Applied Spectroscopy</i> , 2014, 81, 320-327.	0.3	2
6469	Thermodynamic parameters of CdTe crystals in the cubic phase. <i>Journal of Crystal Growth</i> , 2014, 402, 90-93.	0.7	9

#	ARTICLE	IF	CITATIONS
6470	Using Room Temperature Current Noise To Characterize Single Molecular Spectra. ACS Nano, 2014, 8, 2111-2117.	7.3	5
6471	Towards a systematic way to correct density functional approximations. Journal of Chemical Physics, 2014, 140, 18A509.	1.2	12
6472	Symmetry Breaking of $\hat{I}_{\pm}[\text{H}_{2\text{W}}^{12}\text{O}_{40}]^6$ Depends on the Transformation of Isopolyoxotungstates. Inorganic Chemistry, 2014, 53, 5029-5036.	1.9	16
6473	Fluorescent Styryl Dyes Based on Novel 4-Methoxy-9-Methyl-9H-Carbazole-3-Carbaldehyde Synthesis, Photophysical Properties and DFT Computations. Journal of Fluorescence, 2014, 24, 1087-1098.	1.3	5
6474	Kinetics and Mechanism of the Reaction of Fluorine Atoms with Pentafluoropropionic Acid. Journal of Physical Chemistry A, 2014, 118, 4013-4018.	1.1	7
6475	Palladium(II)-Catalyzed Decarboxylative Heck Arylations of Acyclic Electron-Rich Olefins with Internal Selectivity. Advanced Synthesis and Catalysis, 2014, 356, 870-878.	2.1	27
6476	Ring Substituents Mediate the Morphology of PBDTPD-PCBM Bulk-Heterojunction Solar Cells. Chemistry of Materials, 2014, 26, 2299-2306.	3.2	119
6477	Isolation of a Hexanuclear Chromium Cluster with a Tetrahedral Hydridic Core and Its Catalytic Behavior for Ethylene Oligomerization. Inorganic Chemistry, 2014, 53, 6073-6081.	1.9	15
6478	Molecular design of organic dyes with diketopyrrolopyrrole for dye-sensitized solar cell: A theoretical approach. International Journal of Quantum Chemistry, 2014, 114, 560-567.	1.0	16
6479	Synthesis, Structure-Activity, and Structure-Stability Relationships of 2-Substituted-N-(4-oxo-3-oxetanyl)-N-acyl ethanolamine Acid Amidase (NAAA) Inhibitors. ChemMedChem, 2014, 9, 323-336.	1.6	29
6480	Mechanistic Insights into the C-H Bond Activation of Hydrocarbons by Chromium(IV) Oxo and Chromium(III) Superoxo Complexes. Inorganic Chemistry, 2014, 53, 645-652.	1.9	52
6481	Design of a Metal-Organic Framework with Enhanced Back Bonding for Separation of N_2 and CH_4 . Journal of the American Chemical Society, 2014, 136, 698-704.	6.6	157
6482	Density Functional Theory of Open-Shell Systems. The 3d-Series Transition-Metal Atoms and Their Cations. Journal of Chemical Theory and Computation, 2014, 10, 102-121.	2.3	65
6483	Mechanism and kinetic study of 3-fluoropropene with hydroxyl radical reaction. Journal of Molecular Graphics and Modelling, 2014, 48, 18-27.	1.3	10
6484	Effective catalytic disproportionation of aqueous H_2O_2 with di- and mono-nuclear manganese complexes containing pyridine alcohol ligands. Dalton Transactions, 2014, 43, 8599-8608.	1.6	16
6485	On the Pd-C bonding in RPdX and RPdL_2X ($\text{R}=\text{CH}_3, \text{C}_6\text{H}_5$; $\text{L}=\text{PH}_3$; $\text{X}=\text{H}, \text{F}, \text{Cl}, \text{Br}, \text{I}$) compounds. Computational and Theoretical Chemistry, 2014, 1028, 92-97.	1.1	0
6486	Two novel analogous Ni(II) and Cd(II) complexes of an imidazole based Schiff base obtained from imidazole-4-carbaldehyde and 2-aminophenol. Inorganica Chimica Acta, 2014, 409, 399-406.	1.2	9
6487	Density functional and multireference ab initio study of the ground and excited states of Ru2. Chemical Physics Letters, 2014, 592, 24-29.	1.2	11

#	ARTICLE	IF	CITATIONS
6488	PAE113 Peptide: New experimental evidences on its biological activity and conformational insights from molecular dynamics simulations. <i>Biopolymers</i> , 2014, 102, 159-167.	1.2	6
6489	25th Anniversary Article: Design of Polymethine Dyes for All-Optical Switching Applications: Guidance from Theoretical and Computational Studies. <i>Advanced Materials</i> , 2014, 26, 68-84.	11.1	97
6490	Vibrational and Electronic Spectral Study on 3,5-Dihydro-4H-Imidazol-4-One Derivatives Containing Organo-Selenium. <i>Spectroscopy Letters</i> , 2014, 47, 690-703.	0.5	0
6491	A pair of chiral fluorescent sensors for enantioselective recognition of mandelate in water. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 118, 811-815.	2.0	9
6492	A comparative study on properties of two phenoxazine-based dyes for dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2014, 101, 67-73.	2.0	39
6493	Tuning the electron donating ability in the triphenylamine-based D- π -A architecture for highly efficient dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2014, 273, 8-16.	2.0	57
6494	Synthesis, crystal structure and magnetic properties of a novel tetranuclear oxo-bridged iron(III) butterfly. <i>Journal of Molecular Structure</i> , 2014, 1058, 149-154.	1.8	5
6495	Structural Diversity of Copper(I) Complexes Formed by Pyrrole- and Dipyrrolylmethane-Based Diphosphine Ligands with Cu \cdots N-HN Hydrogen Bonds. <i>Inorganic Chemistry</i> , 2014, 53, 700-709.	1.9	27
6496	Origins of Selective C(sp ²) \cdots H Activation Using Transition Metal Complexes with N,N-Bidentate Directing Groups: A Combined Theoretical \cdots Experimental Study. <i>ACS Catalysis</i> , 2014, 4, 649-656.	5.5	51
6497	Thermochemistry, Reaction Paths, and Kinetics on the Secondary Isooctane Radical Reaction with 3 O ₂ . <i>International Journal of Chemical Kinetics</i> , 2014, 46, 71-103.	1.0	8
6498	Biosynthetic consequences of multiple sequential post-transition-state bifurcations. <i>Nature Chemistry</i> , 2014, 6, 104-111.	6.6	128
6499	Huge susceptibility increase within the (1 \cdots x) TeO ₂ +x TeO ₃ crystal system: Ab initio calculation study. <i>Journal of Alloys and Compounds</i> , 2014, 587, 120-125.	2.8	6
6500	Mechanistic Investigations of Palladium-Catalyzed Allylic Fluorination. <i>Organometallics</i> , 2014, 33, 2121-2133.	1.1	63
6501	Nonplanar Donor \cdots Acceptor Chiral Molecules with Large Second-Order Optical Nonlinearities: 1,1,4,4-Tetracyanobuta-1,3-diene Derivatives. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1094-1102.	1.1	15
6502	Benzodithiophene \cdots Thiadiazoloquinoline as an Acceptor for Ambipolar Copolymers with Deep LUMO Level and Distinct Linkage Pattern. <i>Macromolecules</i> , 2014, 47, 979-986.	2.2	41
6503	Polymorph Stability Prediction: On the Importance of Accurate Structures: A Case Study of Pyrazinamide. <i>Crystal Growth and Design</i> , 2014, 14, 381-388.	1.4	19
6504	Following the Molecular Mechanism for the NH ₃ + LiH $\hat{=}$ LiNH ₂ + H ₂ Chemical Reaction: A Study Based on the Joint Use of the Quantum Theory of Atoms in Molecules (QTAIM) and Noncovalent Interaction (NCI) Index. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1663-1672.	1.1	61
6505	Analytical derivative techniques for TDDFT excited-state properties: Theory and application. <i>Science China Chemistry</i> , 2014, 57, 48-57.	4.2	16

#	ARTICLE	IF	CITATIONS
6506	Solvatochromic Fluorescent 2-Substituted 3-Ethynyl Quinoxalines: Four-Component Synthesis, Photophysical Properties, and Electronic Structure. <i>Journal of Organic Chemistry</i> , 2014, 79, 3296-3310.	1.7	70
6507	Formation of Copper Nanoparticles on ZnO Powder by a Surface-Limited Reaction. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1990-1998.	1.5	19
6508	Synthesis of [1,2,4]triazolo[4,3-a]pyrimidin-5(1H)-ones by the Condensation of 3-Alkylamino-5-amino-1-phenyl[1,2,4]triazoles with β -Keto Esters or Diethyl Ethoxymethylenemalonate. <i>Chemistry of Heterocyclic Compounds</i> , 2014, 49, 1500-1507.	0.6	8
6509	Experimental and theoretical studies of the second- and third-order NLO properties of a semi-organic compound: 6-Aminoquinolinium iodide monohydrate. <i>Chemical Physics</i> , 2014, 428, 67-74.	0.9	35
6510	An electron deficient dicyanovinylene-ladder-type pentaphenylene derivative for n-type organic field effect transistors. <i>Journal of Materials Chemistry C</i> , 2014, 2, 3292-3302.	2.7	25
6511	Two-dimensional functional molecular nanoarchitectures – Complementary investigations with scanning tunneling microscopy and X-ray spectroscopy. <i>Progress in Surface Science</i> , 2014, 89, 1-55.	3.8	80
6512	A New-Generation Density Functional. <i>Springer Briefs in Molecular Science</i> , 2014, , .	0.1	20
6513	An application of the reaction class transition state theory to the kinetics of hydrogen abstraction reactions of hydrogen with methyl esters at the methoxy group. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 103-111.	1.1	24
6514	Calculating core-level excitations and x-ray absorption spectra of medium-sized closed-shell molecules with the algebraic diagrammatic construction scheme for the polarization propagator. <i>Journal of Computational Chemistry</i> , 2014, 35, 1900-1915.	1.5	131
6515	Phenalenone Fluorophores-Synthesis, Photophysical Properties and DFT Study. <i>Journal of Fluorescence</i> , 2014, 24, 1827-1840.	1.3	9
6516	Influence of self-assembly on intercalative DNA binding interaction of double-chain surfactant Co(scp) complexes containing imidazo[4,5-f][1,10]phenanthroline and dipyrido[3,2-d:2'-3'-f]quinoxaline ligands: experimental and theoretical study. <i>Dalton Transactions</i> , 2014, 43, 18074-18086.	1.6	41
6517	On the Reaction Mechanism of the Complete Intermolecular O_2 Transfer between Mononuclear Nickel and Manganese Complexes with Macrocyclic Ligands. <i>Chemistry - A European Journal</i> , 2014, 20, 13296-13304.	1.7	7
6518	Modeling of Lead Halide Perovskites for Photovoltaic Applications. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28344-28349.	1.5	143
6519	Predicting Gaseous Reaction Rates of Short Chain Chlorinated Paraffins with H_2O : Overcoming the Difficulty in Experimental Determination. <i>Environmental Science & Technology</i> , 2014, 48, 13808-13816.	4.6	67
6520	Rational modifications on champion porphyrin dye SM315 using different electron-withdrawing moieties toward high performance dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24994-25003.	1.3	40
6521	A perspective on the relative merits of time-dependent and time-independent density functional theory in studies of the electron spectra due to transition metal complexes. An illustration through applications to copper tetrachloride and plastocyanin. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1019-1029.	1.0	24
6522	Crystal Engineering of Tolane Bridged Nitronyl Nitroxide Biradicals: Candidates for Quantum Magnets. <i>Crystal Growth and Design</i> , 2014, 14, 5840-5846.	1.4	11
6523	Quantum Chemical Investigation of Calix[4]arene-Based Radicals with Bis(biphenylene)methyl Linkers as Precursors of Spin Glass and Superparamagnets. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27599-27610.	1.5	7

#	ARTICLE	IF	CITATIONS
6524	Viability of Nonclassical Carbocations Proposed as Intermediates in the Biosynthesis of Atiserene, Beyerene, Kaurene, and Trachylobane Diterpenes. <i>Helvetica Chimica Acta</i> , 2014, 97, 1475-1480.	1.0	6
6525	Double hybrid density functional theory using the coulomb attenuating method. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1199-1211.	1.0	26
6526	Topological \mathbb{Z}_2 -Sn surface states versus film thickness and strain. <i>Physical Review B</i> , 2014, 90, .	1.1	26
6527	Mechanism of Lewis-acid-catalyzed intramolecular coupling of $\text{sp}^3\text{C}-\text{H}$ bond and alkene: A theoretical investigation. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450015.	1.8	0
6528	Geometric structure, electron-energy spectrum, and growth of anionic scandium-silicon clusters ScSi_n^- ($n=6-20$). <i>Journal of Applied Physics</i> , 2014, 116, 124302.	1.1	11
6529	Experimental and Computational Studies of the Ruthenium-Catalyzed Hydrosilylation of Alkynes: Mechanistic Insights into the Regio- and Stereoselective Formation of Vinylsilanes. <i>Organometallics</i> , 2014, 33, 6937-6944.	1.1	58
6530	Gas-Phase Valence-Electron Photoemission Spectroscopy Using Density Functional Theory. <i>Topics in Current Chemistry</i> , 2014, 347, 137-191.	4.0	37
6531	The role of NH_3 and hydrocarbon mixtures in GaN pseudo-halide CVD: a quantum chemical study. <i>Journal of Molecular Modeling</i> , 2014, 20, 2473.	0.8	4
6532	Novel Twisted Intramolecular Charge Transfer (TICT) Extended Fluorescent Styryl Derivatives Containing Quinoline Electron Releasing Moiety. <i>Journal of Fluorescence</i> , 2014, 24, 1811-1825.	1.3	6
6533	A DFT study on the complexation of La^{3+} ion with malonamide and diglycolamide ligands. <i>Russian Journal of Physical Chemistry A</i> , 2014, 88, 2004-2011.	0.1	5
6534	Assessment of approximate computational methods for conical intersections and branching plane vectors in organic molecules. <i>Journal of Chemical Physics</i> , 2014, 141, 124122.	1.2	71
6535	Piecewise Linearity and Spectroscopic Properties from Koopmans-Compliant Functionals. <i>Topics in Current Chemistry</i> , 2014, 347, 193-233.	4.0	19
6536	Impact of Ground and Excited State Aromaticity on Cyclopentadiene and Silole Excitation Energies and Excited State Polarities. <i>Chemistry - A European Journal</i> , 2014, 20, 9295-9303.	1.7	61
6537	Status in Calculating Electronic Excited States in Transition Metal Oxides from First Principles. <i>Topics in Current Chemistry</i> , 2014, 347, 47-98.	4.0	15
6538	Computational Reference Data for the Photochemistry of Cyclobutane Pyrimidine Dimers. <i>ChemPhysChem</i> , 2014, 15, 3342-3354.	1.0	20
6539	Computational Study of van der Waals Complexes between Borylenes and Hydrocarbons. <i>Chemistry - A European Journal</i> , 2014, 20, 12858-12863.	1.7	4
6540	Description of electron transfer in the ground and excited states of organic donor-acceptor systems by single-reference and multi-reference density functional methods. <i>Journal of Chemical Physics</i> , 2014, 141, 124123.	1.2	14
6541	Reasons behind the Relative Abundances of Heptacoordinate Complexes along the Late First-Row Transition Metal Series. <i>Inorganic Chemistry</i> , 2014, 53, 12859-12869.	1.9	35

#	ARTICLE	IF	CITATIONS
6542	The role of zinc in the stability of the marginally stable IscU scaffold protein. <i>Protein Science</i> , 2014, 23, 1208-1219.	3.1	44
6543	Quantum Monte Carlo investigation of the H-shift and O ₂ -loss channels of cis-2-butene-1-peroxy radical. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	0
6544	Main chemical species and molecular structure of deep eutectic solvent studied by experiments with DFT calculation: a case of choline chloride and magnesium chloride hexahydrate. <i>Journal of Molecular Modeling</i> , 2014, 20, 2374.	0.8	37
6545	Theoretical investigation of the mechanisms and dynamics of the reaction CHF ₂ OCHF ₂ Cl+Cl. <i>Journal of Molecular Modeling</i> , 2014, 20, 2419.	0.8	8
6546	An assessment to evaluate the validity of different methods for the description of some corrosion inhibitors. <i>Journal of Molecular Modeling</i> , 2014, 20, 2422.	0.8	10
6547	Self-consistent hybrid functional for condensed systems. <i>Physical Review B</i> , 2014, 89, .	1.1	341
6548	Selective C-H Bond Functionalization of 2-(2-Thienyl)pyridine by a Rhodium N-Heterocyclic Carbene Catalyst. <i>ChemCatChem</i> , 2014, 6, 3192-3199.	1.8	28
6549	C ⁺ Hydrogen Atom Transfer in Post-Cleavage Radical-Cation Complexes: Short and Steep versus Long Winding Road. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10797-10803.	1.1	6
6550	Oxygen Transport in Perovskite-Type Solid Oxide Fuel Cell Materials: Insights from Quantum Mechanics. <i>Accounts of Chemical Research</i> , 2014, 47, 3340-3348.	7.6	121
6551	Calculation of geometric structure, electronic characteristics, vibration frequencies, and thermodynamic properties of C ₁₂ H ₂₀ alkyladamantanes. <i>Petroleum Chemistry</i> , 2014, 54, 270-274.	0.4	2
6552	A prospective DFT study for assembling highly reactive clusters based on lithium boranes and alانات. <i>Molecular Physics</i> , 2014, 112, 316-323.	0.8	5
6553	Simple quinoline-based fluorescent sensor for imaging copper (II) in living cells. <i>Canadian Journal of Chemistry</i> , 2014, 92, 1092-1097.	0.6	13
6554	Catalytic Reactions on the Surface of Ag Nanoparticles: A Photochemical Effect and/or Molecule Property?. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26227-26235.	1.5	24
6555	Hunting the human DPP III active conformation: combined thermodynamic and QM/MM calculations. <i>Dalton Transactions</i> , 2014, 43, 15503-15514.	1.6	22
6556	Computational insight of the mechanism of Algar-Flynn-Oyamada (AFO) reaction. <i>RSC Advances</i> , 2014, 4, 18702.	1.7	17
6557	Luminescence modulation in liquid crystalline phases containing a dispiro[fluorene-9,11-indeno[1,2-b]fluorene-12,9-fluorene] core. <i>Journal of Materials Chemistry C</i> , 2014, 2, 4265-4275.	1.7	20
6558	Receding mechanism of NLO response of polyanion [M ₈ O ₂₆] ⁴⁻ (M = Cr, Mo, W) and the closed loops theory analysis. <i>New Journal of Chemistry</i> , 2014, 38, 2619-2628.	1.4	3
6559	Direct experimental and computational evidence for the dihydride pathway in TangPHOS-Rh catalysed asymmetric hydrogenation. <i>Dalton Transactions</i> , 2014, 43, 1785-1790.	1.6	21

#	ARTICLE	IF	CITATIONS
6560	Formation of hydroxyacetonitrile (HOCH ₂ CN) and polyoxymethylene (POM)-derivatives in comets from formaldehyde (CH ₂ O) and hydrogen cyanide (HCN) activated by water. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 3360-3370.	1.3	36
6561	A successful DFT calculation of carbon-13 NMR chemical shifts and carbon-fluorine spin-spin coupling constants in (η ⁶ -fluoroarene)tricarbonylchromium complexes. <i>RSC Advances</i> , 2014, 4, 27290-27296.	1.7	15
6562	Ligand spheres in asymmetric hetero Diels-Alder reactions catalyzed by Cu(II) box complexes: experiment and modeling. <i>Dalton Transactions</i> , 2014, 43, 698-705.	1.6	10
6563	Symmetrically Disubstituted Bithiophene Derivatives of 1,3,4-Oxadiazole, 1,3,4-Thiadiazole, and 1,2,4-Triazole – Spectroscopic, Electrochemical, and Spectroelectrochemical Properties. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25176-25189.	1.5	33
6564	Improvements in DFT Calculations of Spin-Spin Coupling Constants. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4938-4949.	2.3	31
6565	Organotin bond dissociation energies: An interesting challenge for contemporary computational methods. <i>Computational and Theoretical Chemistry</i> , 2014, 1050, 7-14.	1.1	10
6566	C-H and C-O bond activation with a rhodium(I) η ² -diiminate complex. <i>Dalton Transactions</i> , 2014, 43, 11286.	1.6	5
6567	Excited states using the simplified Tamm-Dancoff-Approach for range-separated hybrid density functionals: development and application. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14408-14419.	1.3	76
6568	Molecular design of organic sensitizers absorbing over a broadened visible region for dye-sensitized solar cells. <i>RSC Advances</i> , 2014, 4, 57916-57922.	1.7	5
6569	Unimolecular reaction chemistry of a charge-tagged beta-hydroxyperoxyl radical. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24954-24964.	1.3	9
6570	Formaldehyde chemistry in cometary ices: the case of HOCH ₂ OH formation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24200-24208.	1.3	21
6571	New organic dyes based on a dibenzofulvene bridge for highly efficient dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2014, 2, 14181-14188.	5.2	31
6572	In-depth exploration of the photophysics of a trinuclear palladium complex. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 8332-8338.	1.3	10
6573	Charting the mechanism and reactivity of zirconium oxalate with hydroxamate ligands using density functional theory: implications in new chelate design. <i>Dalton Transactions</i> , 2014, 43, 9872-9884.	1.6	44
6574	Quantum rules for planar boron nanoclusters. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18311-18318.	1.3	33
6575	Adsorption of CO, SO ₂ , HCN, NH ₃ , and H ₂ CO on zigzag GaP nanotubes: a QM/MM study. <i>RSC Advances</i> , 2014, 4, 59056-59063.	1.7	7
6576	Role of hydrogen bonds in molecular packing of photoreactive crystals: templating photodimerization of protonated stilbazoles in crystalline state with a combination of water molecules and chloride ions. <i>Photochemical and Photobiological Sciences</i> , 2014, 13, 1509-1520.	1.6	15
6577	An investigation of possible competing mechanisms for Ni-containing methyl-coenzyme M reductase. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14029.	1.3	28

#	ARTICLE	IF	CITATIONS
6578	DFT Study of Reduction Mechanisms of Ethylene Carbonate and Fluoroethylene Carbonate on Li ⁺ -Adsorbed Si Clusters. <i>Journal of the Electrochemical Society</i> , 2014, 161, E3097-E3109.	1.3	36
6579	Docking and molecular dynamics studies of the binding between Peloruside A and tubulin. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2014, 29, 702-709.	2.5	3
6580	A First-Principles Approach to the Calculation of the on-Site Zero-Field Splitting in Polynuclear Transition Metal Complexes. <i>Inorganic Chemistry</i> , 2014, 53, 11785-11793.	1.9	32
6581	Quantum-chemical insights into mixed-valence systems: within and beyond the Robin-Day scheme. <i>Chemical Society Reviews</i> , 2014, 43, 5067-5088.	18.7	168
6582	Charge self-localization in π -conjugated polymers by long range corrected hybrid functionals. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6700.	1.3	9
6583	An Insight into Prototropism and Supramolecular Motifs in Solid-State Structures of Allopurinol, Hypoxanthine, Xanthine, and Uric Acid. ^1H - ^{14}N NQDR Spectroscopy, Hybrid DFT/QTAIM, and Hirshfeld Surface-Based Study. <i>Journal of Physical Chemistry B</i> , 2014, 118, 10837-10853.	1.2	18
6584	Pentalenene formation mechanisms redux. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 887-894.	1.5	24
6585	Photophysics of Flavin Derivatives Absorbing in the Blue-Green Region: Thioflavins As Potential Cofactors of Photoswitches. <i>Journal of Physical Chemistry B</i> , 2014, 118, 1743-1753.	1.2	18
6586	Mercury Oxidation via Chlorine, Bromine, and Iodine under Atmospheric Conditions: Thermochemistry and Kinetics. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2959-2975.	1.1	41
6587	Benchmark Many-Body <i>GW</i> and Bethe-Salpeter Calculations for Small Transition Metal Molecules. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3934-3943.	2.3	98
6588	Torque-selective Ring Opening of Fused Cyclobutenamides: Evidence for a <i>Cis,Trans</i> -Cyclooctadienone Intermediate. <i>Journal of the American Chemical Society</i> , 2014, 136, 9802-9805.	6.6	27
6589	Graphitic Silicon Nitride: A Metal-Free Ferromagnet with Charge and Spin Current Rectification. <i>ChemPhysChem</i> , 2014, 15, 2756-2761.	1.0	8
6590	Direct Spectroscopic Evidence for Constituent Heteroatoms Enhancing Charge Recombination at a TiO_2 -Ruthenium Dye Interface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17079-17089.	1.5	20
6591	Revisiting the role of exact exchange in DFT spin-state energetics of transition metal complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14479-14488.	1.3	68
6592	Optical excitation of MgO nanoparticles; a computational perspective. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22052-22061.	1.3	33
6593	Characterization of one-electron oxidized copper(II)-salophen-type complexes; effects of electronic and geometrical structures on reactivities. <i>Dalton Transactions</i> , 2014, 43, 2283-2293.	1.6	45
6594	Stability of ruthenium/organic dye co-sensitized solar cells: a joint experimental and computational investigation. <i>RSC Advances</i> , 2014, 4, 57620-57628.	1.7	14
6595	Theoretical calculations of the kinetics of the OH reaction with 2-methyl-2-propen-1-ol and its alkene analogue. <i>RSC Advances</i> , 2014, 4, 20830-20840.	1.7	8

#	ARTICLE	IF	CITATIONS
6596	Structures and properties of coordination polymers involving asymmetric biphenyl-3,2,5-tricarboxylate. <i>CrystEngComm</i> , 2014, 16, 10006-10016.	1.3	16
6597	Muon Radiolysis Affected by Density Inhomogeneity in Near-Critical Fluids. <i>Radiation Research</i> , 2014, 181, 396-406.	0.7	4
6598	Computational study of the working mechanism and rate acceleration of overcrowded alkene-based light-driven rotary molecular motors. <i>RSC Advances</i> , 2014, 4, 10240.	1.7	21
6599	Mechanisms and Reactivity Differences for Cycloaddition of Anhydride to Alkyne Catalyzed by Palladium and Nickel Catalysts: Insight from Density Functional Calculations. <i>Journal of Organic Chemistry</i> , 2014, 79, 11911-11921.	1.7	32
6600	Electrochemical reduction of N,N'-thiobisphthalimide and N,N'-dithiobisphthalimide: ejection of diatomic sulfur through an autocatalytic mechanism. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22600-22610.	1.3	1
6601	Secondary stereocontrolling interactions in chiral Brønsted acid catalysis: study of a Petasis-Ferrier-type rearrangement catalyzed by chiral phosphoric acids. <i>Chemical Science</i> , 2014, 5, 3515-3523.	3.7	55
6602	The structural origin of the unusual compression behaviors in nanostructured TiO ₂ : insights from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18156-18162.	1.3	3
6603	Coupled-cluster calculations of the lowest O ² bands of the electronic excitation spectrum of naphthalene. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9859.	1.3	15
6604	An inelastic neutron scattering study of dietary phenolic acids. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7491-7500.	1.3	10
6605	Dual mode of extraction for Cs ⁺ and Na ⁺ ions with dicyclohexano-18-crown-6 and bis(2-propyloxy)calix[4]crown-6 in ionic liquids: density functional theoretical investigation. <i>RSC Advances</i> , 2014, 4, 22911-22925.	1.7	31
6606	The derivative discontinuity of the exchange-correlation functional. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14378-14387.	1.3	74
6607	Kinetic Effects of Sulfur Oxidation on Catalytic Nitrile Hydration: Nitrile Hydratase Insights from Bioinspired Ruthenium(II) Complexes. <i>Inorganic Chemistry</i> , 2014, 53, 12372-12377.	1.9	15
6608	Palladium Complexes with Chelating Bis-NHC Ligands in the Mizoroki-Heck Reaction Mechanism and Electronic Effects, a DFT Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 12096-12105.	1.7	35
6609	Relating polarizability to volume, ionization energy, electronegativity, hardness, moments of momentum, and other molecular properties. <i>Journal of Chemical Physics</i> , 2014, 141, 074306.	1.2	57
6610	Variational, Self-Consistent Implementation of the Perdew-Zunger Self-Interaction Correction with Complex Optimal Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5324-5337.	2.3	69
6611	Theoretical studies on the quinoidal thiophene based dyes for dye sensitized solar cell and NLO applications. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21496-21505.	1.3	30
6612	P-H activation of secondary phosphanes on a parent amido diiridium complex. <i>Dalton Transactions</i> , 2014, 43, 1609-1619.	1.6	18
6613	The one-electron reduction of dithiolate and diselenolate ligands. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10897.	1.3	11

#	ARTICLE	IF	CITATIONS
6614	Non-innocent side-chains with dipole moments in organic solar cells improve charge separation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12454-12461.	1.3	21
6615	Limiting nuclearity in formation of polynuclear metal complexes through [2 + 3] cycloaddition: synthesis and magnetic properties of tri- and pentanuclear metal complexes. <i>Dalton Transactions</i> , 2014, 43, 8083-8093.	1.6	13
6616	Palladium(II)-Catalyzed Desulfitative Synthesis of Aryl Ketones from Sodium Arylsulfonates and Nitriles: Scope, Limitations, and Mechanistic Studies. <i>Journal of Organic Chemistry</i> , 2014, 79, 12018-12032.	1.7	63
6617	Thermal and solvent effects on the triplet formation in cinnoline. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4740.	1.3	61
6618	A partial differential equation for pseudocontact shift. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20184-20189.	1.3	35
6619	A RRKM study and a DFT assessment on gas-phase fragmentation of formamide ^{M2+} (M = Ca, Sr). <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14813.	1.3	7
6620	High nuclearity Ni(ⁱⁱ) cages from hydroxamate ligands. <i>RSC Advances</i> , 2014, 4, 38182-38191.	1.7	15
6621	A simple BODIPY-aniline-based fluorescent chemosensor as multiple logic operations for the detection of pH and CO ₂ gas. <i>Dalton Transactions</i> , 2014, 43, 8499-8507.	1.6	71
6622	Aromatic fused heterocyclic [22] macrocycles with NIR absorption. <i>Chemical Communications</i> , 2014, 50, 9094.	2.2	14
6623	Fast and reversible insertion of carbon dioxide into zirconocene ^{alkoxide} bonds. A mechanistic study. <i>Dalton Transactions</i> , 2014, 43, 8894-8898.	1.6	4
6624	Effect of charge transfer and periodicity on the magnetism of [Cr(Cp [*]) ₂][ETCE]. <i>RSC Advances</i> , 2014, 4, 14847.	1.7	1
6625	Sequential carboxylation/intramolecular cyclization reaction of o-alkynyl acetophenone with CO ₂ . <i>Organic Chemistry Frontiers</i> , 2014, 1, 275.	2.3	40
6626	Interstellar H adsorption and H ₂ formation on the crystalline (010) forsterite surface: a B3LYP-D2* periodic study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17447-17457.	1.3	28
6627	Conformational and zwitterionic preferences of N-amidinoglycine: the effect of microsolvation and metal ion addition. <i>RSC Advances</i> , 2014, 4, 45332-45344.	1.7	3
6628	A theoretical study of the nornicotine-catalyzed Mannich reaction in wet solvents and water. <i>Green Chemistry</i> , 2014, 16, 3999-4008.	4.6	6
6629	Photoinduced solid state keto ^{enol} tautomerization of 2-(2-(3-nitrophenyl)-4,5-diphenyl-1H-imidazol-1-yloxy)-1-phenylethanone. <i>RSC Advances</i> , 2014, 4, 8044.	1.7	6
6630	One-electron self-interaction and the asymptotics of the Kohn ^{Sham} potential: an impaired relation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14357-14367.	1.3	56
6631	Design of coordination polymers with 4 ² -substituted functionalized terpyridyls in the backbone and pendent cyclopentadienyliron moieties. <i>Polymer Chemistry</i> , 2014, 5, 3453-3465.	1.9	23

#	ARTICLE	IF	CITATIONS
6632	Exploring the mechanism of Grignard metathesis polymerization of 3-alkylthiophenes. Dalton Transactions, 2014, 43, 15143-15150.	1.6	38
6633	Substituted diphenyl butadiynes: a computational study of geometries and electronic transitions using DFT/TD-DFT. Physical Chemistry Chemical Physics, 2014, 16, 14015.	1.3	26
6634	Mechanistic insight into the hydroxylation of alkanes by a nonheme iron(IV)=O complex. Chemical Communications, 2014, 50, 5572-5575.	2.2	67
6635	Reaction mechanism and free energy profile for acylation of <i>Candida Antarctica</i> lipase B with methylcaprylate and acetylcholine: Density functional theory calculations. Journal of Molecular Graphics and Modelling, 2014, 54, 131-140.	1.3	10
6636	A dominant homolytic O–Cl bond cleavage with low-spin triplet-state Fe(IV)=O formed is revealed in the mechanism of heme-dependent chlorite dismutase. Dalton Transactions, 2014, 43, 973-981.	1.6	21
6637	A stable, mononuclear, cationic Pt(IV) complex stabilised by bulky N-heterocyclic carbenes. Chemical Communications, 2014, 50, 1299-1301.	2.2	21
6638	A complete scheme of tautomerism on diacetyl monoxime in the gas and solution phases. A comparative DFT study between B3LYP and M06-2X functionals. Computational and Theoretical Chemistry, 2014, 1045, 10-21.	1.1	23
6639	Facilitating the Cope Rearrangement by Partial Protonation: Implications for Synthesis and Biosynthesis. Organic Letters, 2014, 16, 4818-4821.	2.4	8
6640	Molecular Dynamics Simulation Study of Methanesulfonic Acid. Journal of Physical Chemistry B, 2014, 118, 3423-3430.	1.2	6
6641	Characterization of the Bridged Hyponitrite Complex $\{[\text{Fe}(\text{OEP})]_2(\mu_4\text{-N}_2\text{O}_2)\}$: Reactivity of Hyponitrite Complexes and Biological Relevance. Inorganic Chemistry, 2014, 53, 6398-6414.	1.9	42
6642	Theoretical study on the static and dynamic first-order hyperpolarisabilities of adenine tautomers. Molecular Physics, 2014, 112, 1755-1760.	0.8	5
6643	Unsymmetrical squaraine dye containing dithieno[3,2-b:2',3'-d]pyrrole as a spacer: A potential photosensitizer for dye-sensitized solar cells. Journal of Power Sources, 2014, 268, 137-145.	4.0	22
6644	Benzothiazoline Three-Coordinated Organoboron Compounds with a B–N Bond: Dual Emission and Temperature-Dependent Excimer Fluorescence. Organometallics, 2014, 33, 5483-5491.	1.1	13
6645	Ligand Effects on the Regioselectivity of Rhodium-Catalyzed Hydroformylation: Density Functional Calculations Illuminate the Role of Long-Range Noncovalent Interactions. Organometallics, 2014, 33, 4183-4191.	1.1	47
6646	Theoretical prediction of structural, vibrational and NMR parameters of plastic optical fiber (POF) material precursors. Cis and trans perhydro- and perfluoro-2-methylene-4,5-dimethyl-1,3-dioxolanes. Journal of Molecular Graphics and Modelling, 2014, 52, 36-45.	1.3	5
6647	Modification of the Configuration toward a High-Performance Triphenylamine-Based Sensitizer for Dye-Sensitized Solar Cells: A Theoretical Investigation. ChemPhysChem, 2014, 15, 3809-3818.	1.0	16
6648	Computational Investigation of Alkynols and Alkyndiols Hydrogenation on a Palladium Cluster. Journal of Physical Chemistry C, 2014, 118, 551-558.	1.5	19
6649	Reaction Mechanism of Homoprotocatechuate 2,3-Dioxygenase with 4-Nitrocatechol: Implications for the Role of Substrate. Journal of Physical Chemistry B, 2014, 118, 1791-1798.	1.2	27

#	ARTICLE	IF	CITATIONS
6650	Novel Capsaicin Analogues as Potential Anticancer Agents: Synthesis, Biological Evaluation, and <i>In Silico</i> Approach. <i>Archiv Der Pharmazie</i> , 2014, 347, 885-895.	2.1	14
6651	Resonance IR: A Coherent Multidimensional Analogue of Resonance Raman. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3112-3119.	1.1	17
6652	Hydroxylated Derivatives of NPC1161: Theoretical Insights into Their Potential Toxicity and the Feasibility and Regioselectivity of Their Formation. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5501-5507.	1.1	4
6653	Nickel(II) Complexes of Pentadentate N5 Ligands as Catalysts for Alkane Hydroxylation by Using <i>m</i> -CPBA as Oxidant: A Combined Experimental and Computational Study. <i>Chemistry - A European Journal</i> , 2014, 20, 11346-11361.	1.7	72
6654	Catalytic Effect of Water, Formic Acid, or Sulfuric Acid on the Reaction of Formaldehyde with OH Radicals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4797-4807.	1.1	82
6655	Rationalization of the pK_a Values of Alcohols and Thiols Using Atomic Charge Descriptors and Its Application to the Prediction of Amino Acid pK_a 's. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2200-2213.	2.5	58
6656	Theoretical Study of the Gas-Phase Reactions of NO ₃ Radical with a Series of <i>trans</i> -2-Unsaturated Aldehydes: From Acrolein to <i>trans</i> -2-Octenal. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5149-5155.	1.1	15
6657	Phenyl- and Thienyl-Ended Symmetric Azomethines and Azines as Model Compounds for n-Channel Organic Field-Effect Transistors: An Electrochemical and Computational Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3984-3993.	1.5	30
6658	Monte Carlo Modeling of Carbon Dioxide Adsorption in Porous Aromatic Frameworks. <i>Langmuir</i> , 2014, 30, 4147-4156.	1.6	19
6659	Characteristic Spectral Patterns in the Carbon-13 Nuclear Magnetic Resonance Spectra of Hexagonal and Crenellated Graphene Fragments. <i>ChemPhysChem</i> , 2014, 15, 1799-1808.	1.0	11
6660	Interfacial Properties and Design of Functional Energy Materials. <i>Accounts of Chemical Research</i> , 2014, 47, 3395-3405.	7.6	14
6661	Manipulating Magnetism: Ru ₂ ⁵⁺ Paddlewheels Devoid of Axial Interactions. <i>Journal of the American Chemical Society</i> , 2014, 136, 9580-9589.	6.6	24
6662	An Integrated Experimental and Theoretical Approach to the Spectroscopy of Organic Dye-Sensitized TiO ₂ Heterointerfaces: Disentangling the Effects of Aggregation, Solvation, and Surface Protonation. <i>ChemPhysChem</i> , 2014, 15, 1116-1125.	1.0	26
6663	Experimental and Quantum Chemical Modeling Studies of the Interactions of <i>L</i> -Phenylalanine with Divalent Transition Metal Cations. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2524-2535.	2.5	13
6664	Synthesis, X-ray structural features, DFT calculations and fluorescence studies of a new pyridoxal-benzimidazole ligand and its respective molybdenum complex. <i>New Journal of Chemistry</i> , 2014, 38, 3092-3101.	1.4	6
6665	Electronic descriptors for analytical use of the benzidine-based compounds and the mechanism of oxidative coupling of anilines. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 640-651.	0.9	11
6666	Copper Coordination Study in a Metal-Induced Chiral Polythiophene Aggregate. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9769-9779.	1.5	4
6667	DNA/protein interaction and cytotoxic activity of imidazole terpyridine derived Cu(II)/Zn(II) metal complexes. <i>Dalton Transactions</i> , 2014, 43, 13018.	1.6	69

#	ARTICLE	IF	CITATIONS
6668	Theoretical Study on the Kinetics of the Reaction $\text{CH}_2\text{Br} + \text{NO}_2$. Journal of Physical Chemistry A, 2014, 118, 3313-3318.	1.1	4
6669	Synthesis of Dawson-Type Silicotungstate $[\text{Si}_2\text{W}_{18}\text{O}_{62}]^{8-}$ and Protonation and Deprotonation Inside the Aperture through Intramolecular Hydrogen Bonds. Chemistry - A European Journal, 2014, 20, 5946-5952.	1.7	43
6670	Solution structures of purine base analogues 6-chloroguanine, 8-azaguanine and allopurinol. Journal of Biomolecular Structure and Dynamics, 2014, 32, 27-35.	2.0	6
6671	Mechanistic Investigation of Dirhodium-Catalyzed Intramolecular Allylic C-H Amination versus Alkene Aziridination. Journal of Organic Chemistry, 2014, 79, 9799-9811.	1.7	48
6672	Nitrogen-doped porous carbon monolith as a highly efficient catalyst for CO_2 conversion. Journal of Materials Chemistry A, 2014, 2, 18360-18366.	5.2	75
6673	Reactivities of Substituted <i>tert</i> -butyl Nitrones. Journal of Organic Chemistry, 2014, 79, 6615-6626.	1.7	21
6674	Multilithiation Effect on the First Hyperpolarizability of Carbon-Boron-Nitride Heteronanotubes: Activating Segment versus Connecting Pattern. Journal of Physical Chemistry C, 2014, 118, 14185-14191.	1.5	33
6675	Large Hyperconjugation in Strained Systems. Chemistry - A European Journal, 2014, 20, 12601-12606.	1.7	8
6676	A dispersion-corrected DFT study on adsorption of battery active materials anthraquinone and its derivatives on monolayer graphene and h-BN. Journal of Materials Chemistry A, 2014, 2, 8910-8917.	5.2	115
6677	Density functional study on the effect of a new ladder-type structure with different substituent groups ($\text{R} = \text{H}, \text{CH}_3, \text{OCH}_3$ and CN) for donor-acceptor copolymers. RSC Advances, 2014, 4, 36656.	1.7	4
6678	Benchmarking dispersion and geometrical counterpoise corrections for cost-effective large-scale DFT calculations of water adsorption on graphene. Journal of Computational Chemistry, 2014, 35, 1789-1800.	1.5	24
6679	Deconstructing the Catalytic Efficiency of Peroxiredoxin-5 Peroxidatic Cysteine. Biochemistry, 2014, 53, 6113-6125.	1.2	63
6680	Ab initio chemical kinetics for the $\text{N}_2\text{H}_4 + \text{NO}$ ($\chi = 1-3$) reactions and related reverse processes. Computational and Theoretical Chemistry, 2014, 1046, 73-80.	1.1	6
6681	New Organic Donor-Acceptor-Acceptor Sensitizers for Efficient Dye-Sensitized Solar Cells and Photocatalytic Hydrogen Evolution under Visible-Light Irradiation. ChemSusChem, 2014, 7, 2879-2888.	3.6	50
6682	Lifetimes of carbocations encountered along reaction coordinates for terpene formation. Chemical Science, 2014, 5, 3301.	3.7	33
6683	Density Differences in Embedding Theory with External Orbital Orthogonality. Journal of Physical Chemistry A, 2014, 118, 9182-9200.	1.1	36
6684	TeO_2 nanostructures as a NO_2 sensor: DFT investigation. Computational and Theoretical Chemistry, 2014, 1049, 20-27.	1.1	42
6685	Unraveling the Pivotal Impacts of Electron-Acceptors on Light Absorption and Carrier Photogeneration in Perylene Dye Sensitized Solar Cells. ACS Photonics, 2014, 1, 710-717.	3.2	34

#	ARTICLE	IF	CITATIONS
6686	Catalyst activation and the dimerization energy of alkylaluminium compounds. <i>Journal of Organometallic Chemistry</i> , 2014, 772-773, 161-171.	0.8	59
6687	Molecular size from moments of the momentum density. <i>Chemical Physics Letters</i> , 2014, 609, 113-116.	1.2	7
6688	Kinetics and mechanism of the water-assisted reaction of NCO with CH ₃ OH: A quantum chemical study. <i>Computational and Theoretical Chemistry</i> , 2014, 1044, 55-61.	1.1	5
6689	Ab Initio Treatment of Disorder Effects in Amorphous Organic Materials: Toward Parameter Free Materials Simulation. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3720-3725.	2.3	106
6690	Effect of a Long Alkyl Group on Cyclopentadithiophene as a Conjugated Bridge for Organic Sensitizers: IPCE, Electron Diffusion Length, and Charge Recombination. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 14621-14630.	4.0	67
6691	Theoretical unification of hybrid-DFT and $\langle \text{DFT} \rangle$ for the treatment of localized orbitals. <i>Physical Review B</i> , 2014, 90, .		
6692	Theoretical study on a corrole-azafullerene dyad: Electronic structure, spectra and photoinduced electron transfer. <i>Chemical Physics Letters</i> , 2014, 610-611, 50-55.	1.2	4
6693	Novel tacrine/acridine anticholinesterase inhibitors with piperazine and thiourea linkers. <i>International Journal of Biological Macromolecules</i> , 2014, 70, 435-439.	3.6	38
6694	DFT cluster model study of MoVO-type mixed-metal oxides. <i>Computational and Theoretical Chemistry</i> , 2014, 1045, 57-65.	1.1	7
6695	Performance of exchange-correlation functionals on describing ground state geometries and excitations of Alizarin Red S: Effect of complexation and degree of deprotonation. <i>Computational and Theoretical Chemistry</i> , 2014, 1045, 113-122.	1.1	9
6696	The exceptions to the Walsh rules: Linear and cyclic structures of EX ₂ (E=C, Si, Ge, Sn, Pb and X=O, S).	1.1	5
6697	Additive models for the molecular polarizability and volume. <i>Chemical Physics Letters</i> , 2014, 610-611, 163-166.	1.2	20
6698	Performance of the M06 family of functionals in prediction of the charge transfer transition energies of the naphthalene-TCNE and pyrene-TCNE molecular complexes. <i>Chemical Physics Letters</i> , 2014, 610-611, 19-22.	1.2	9
6699	Comprehensive Analysis of Gly-Leu-Gly-Gly-Lys Peptide Dication Structures and Cation-Radical Dissociations Following Electron Transfer: From Electron Attachment to Backbone Cleavage, Ion-Molecule Complexes, and Fragment Separation. <i>Journal of Physical Chemistry A</i> , 2014, 118, 308-324.	1.1	26
6700	Electrostatic Potential within the Free Volume Space of Imidazole-Based Solvents: Insights into Gas Absorption Selectivity. <i>Journal of Physical Chemistry B</i> , 2014, 118, 255-264.	1.2	26
6701	Unraveling the Electronic Structure of Azolehemiporphyrines: Direct Spectroscopic Observation of Magnetic Dipole Allowed Nature of the Lowest $\pi \rightarrow \pi^*$ Transition of 20-Electron Porphyrinoids. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4415-4424.	1.1	15
6702	Benchmarking DFT and TD-DFT Functionals for the Ground and Excited States of Hydrogen-Rich Peptide Radicals. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3308-3318.	2.3	33
6703	Quantum-Chemical Insight into Structure-Reactivity Relationship in 4,5,6,7-Tetrahalogeno-1 <i>H</i> -benzimidazoles: A Combined X-ray, DSC, DFT/QAIM, Hirshfeld Surface-Based, and Molecular Docking Approach. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2089-2106.	1.1	22

#	ARTICLE	IF	CITATIONS
6704	Long-lived Trifluoromethanide Anion: A Key Intermediate in Nucleophilic Trifluoromethylations. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 11575-11578.	7.2	122
6705	Theoretical Studies on the Mechanism, Enantioselectivity, and Axial Ligand Effect of a Ru(salen)-Catalyzed Asymmetric Cyclopropanation Reaction. <i>Organometallics</i> , 2014, 33, 3673-3682.	1.1	14
6706	Examining the Amine Functionalization in Dicarboxylates: Photoelectron Spectroscopy and Theoretical Studies of Aspartate and Glutamate. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5256-5262.	1.1	5
6707	Multivalency of Group 15 Dopants in SnO ₂ . <i>Chemistry of Materials</i> , 2014, 26, 4876-4881.	3.2	11
6708	Organic-based magnetic semiconductor thin film of Fe(TCNQ) ^{1/2} developed by physical vapor deposition and local spin density induced core-level shifts. <i>Synthetic Metals</i> , 2014, 196, 56-60.	2.1	2
6709	DFT study on IR spectral and structural changes caused by the conversion of substituted benzophenones into ketyl radicals. <i>Computational and Theoretical Chemistry</i> , 2014, 1046, 57-63.	1.1	6
6710	The Variationally Orbital-Adapted Configuration Interaction Singles (VOA-CIS) Approach to Electronically Excited States. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1004-1020.	2.3	36
6711	Investigating Superoxide Transfer through a $\mu_4-1,2-O_2$ Bridge between Nonheme Ni ^{III} -Peroxo and Mn ^{II} Species by DFT Methods to Bridge Theoretical and Experimental Views. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2437-2442.	2.1	7
6712	Benchmark Study on Methanol C-H and O-H Bond Activation by Bare [Fe ^{IV} O] ²⁺ . <i>Journal of Physical Chemistry A</i> , 2014, 118, 7146-7158.	1.1	30
6713	PdCl ₂ on modified poly(styrene-co-maleic anhydride): A highly active and recyclable catalyst for the Suzuki-Miyaura and Sonogashira reactions. <i>Journal of Molecular Catalysis A</i> , 2014, 394, 74-82.	4.8	86
6714	Mechanism for covalence bond benzene dimers formation: A DFT and MP2 investigation. <i>Chemical Physics Letters</i> , 2014, 610-611, 192-197.	1.2	5
6715	meso-C6F5 substituted BODIPYs with distinctive spectroscopic properties and their application for bioimaging in living cells. <i>Tetrahedron</i> , 2014, 70, 5800-5805.	1.0	23
6716	Interaction of anthranilic acid with silver nanoparticles: A Raman, surface-enhanced Raman scattering and density functional theoretical study. <i>Journal of Molecular Structure</i> , 2014, 1076, 35-41.	1.8	18
6717	Synthesis, X-ray diffraction analysis and nonlinear optical properties of hexacoordinated organotin compounds derived from Schiff bases. <i>Journal of Organometallic Chemistry</i> , 2014, 769, 64-71.	0.8	28
6718	The Catalytic Mechanism of Carboxylesterases: A Computational Study. <i>Biochemistry</i> , 2014, 53, 5820-5829.	1.2	53
6719	The benzoin condensation: Charge tagging of the catalyst allows for tracking by mass spectrometry. <i>International Journal of Mass Spectrometry</i> , 2014, 369, 92-97.	0.7	8
6720	The effect of polyaromatic hydrocarbons on the spectral and photophysical properties of diaryl-pyrrole derivatives: an experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18319.	1.3	6
6721	Indanthrone dye revisited after sixty years. <i>Chemical Communications</i> , 2014, 50, 11543-11546.	2.2	25

#	ARTICLE	IF	CITATIONS
6722	Multiscale Modelling of Organic and Hybrid Photovoltaics. <i>Topics in Current Chemistry</i> , 2014, , .	4.0	24
6723	Exploring the topography of the stress-modified energy landscapes of mechanosensitive molecules. <i>Journal of Chemical Physics</i> , 2014, 140, 104114.	1.2	41
6724	Theoretical Study on the Reaction of the Methylidyne Radical, CH(X ²), with Formaldehyde, CH ₂ O. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8861-8871.	1.1	9
6725	Ultrafast C _{spiro} O Dissociation via a Conical Intersection Drives Spiropyran to Merocyanine Photoswitching. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1339-1349.	1.1	47
6726	Double-hybrid density functionals. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 576-600.	6.2	292
6727	Organic Dyes Containing Carbazole as Donor and π -Linker: Optical, Electrochemical, and Photovoltaic Properties. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 2528-2539.	4.0	170
6728	A New Tool To Guide Halofunctionalization Reactions: The Halenium Affinity (<i>HalA</i>) Scale. <i>Journal of the American Chemical Society</i> , 2014, 136, 13355-13362.	6.6	77
6729	Performance of Density Functional Theory Procedures for the Calculation of Proton-Exchange Barriers: Unusual Behavior of M06-Type Functionals. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3777-3783.	2.3	44
6730	Fragmentation of Peptide Radical Cations Containing a Tyrosine or Tryptophan Residue: Structural Features That Favor Formation of [X _n + H] ⁺ and [Z _n + H] ⁺ Ions. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6123-6133.	1.2	11
6731	Spatial structure and electronic spectrum of TiSi _n clusters (n = 6-18). <i>Russian Journal of Physical Chemistry A</i> , 2014, 88, 1712-1718.	0.1	3
6732	Maximizing the Electromagnetic and Chemical Resonances of Surface-Enhanced Raman Scattering for Nucleic Acids. <i>ACS Nano</i> , 2014, 8, 8383-8391.	7.3	28
6733	Electrocyclic [1,5] hydrogen shift in the thermal elimination kinetics of phenyl acetate and <i>p</i> -tolyl acetate in the gas phase: a density functional theory study. <i>Molecular Physics</i> , 2014, 112, 462-473.	0.8	6
6734	Theoretical Studies on the Mechanism of Iridium-Catalyzed Alkene Hydrogenation by the Cationic Complex [IrH ₂ (NCMe) ₃ (P ₃)] ⁺ . <i>Organometallics</i> , 2014, 33, 5156-5163.	1.1	23
6735	First-Principles Calculations of the Pressure Stability and Elasticity of Dense TiO ₂ Phases Using the B3LYP Hybrid Functional. <i>Journal of Physical Chemistry C</i> , 2014, 118, 8617-8625.	1.5	20
6736	Hybrid Density Functionals for Clusters of Late Transition Metals: Assessing Energetic and Structural Properties. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4408-4416.	2.3	21
6737	Calculating X-ray Absorption Spectra of Open-Shell Molecules with the Unrestricted Algebraic-Diagrammatic Construction Scheme for the Polarization Propagator. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4583-4598.	2.3	80
6738	Optimizing Calculations of Electronic Excitations and Relative Hyperpolarizabilities of Electrooptic Chromophores. <i>Accounts of Chemical Research</i> , 2014, 47, 3258-3265.	7.6	164
6739	Design of D-A organic dyes with different acceptor and auxiliary acceptor for highly efficient dye-sensitized solar cells: a computational study. <i>RSC Advances</i> , 2014, 4, 50338-50350.	1.7	43

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6740	DFT Investigation of Formaldehyde Adsorption Characteristics on MgO Nanotube. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2014, 24, 1038-1047.	1.9	24
6741	Functional tuning of phenothiazine-based dyes by a benzimidazole auxiliary chromophore: an account of optical and photovoltaic studies. <i>RSC Advances</i> , 2014, 4, 53588-53601.	1.7	35
6742	Analysis of Stereochemistry Control in Homogeneous Olefin Polymerization Catalysis. <i>Organometallics</i> , 2014, 33, 5974-5982.	1.1	24
6743	Imidazolium-based ionic liquids with different fatty acid anions: phase behavior, electronic structure and ionic conductivity investigation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16255.	1.3	35
6744	Exciton Circular Dichroism in Channelrhodopsin. <i>Journal of Physical Chemistry B</i> , 2014, 118, 11873-11885.	1.2	12
6745	Reactions of Methanol with Pristine and Defective Ceria (111) Surfaces: A Comparison of Density Functionals. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23690-23700.	1.5	33
6746	Theoretical study on the mechanism of CH ₃ NH ₂ and O ₃ atmospheric reaction. <i>Journal of Chemical Sciences</i> , 2014, 126, 1173-1180.	0.7	4
6747	First principle study of the sensitivity of CO adsorption on pure and binary clusters of lead and silicon. <i>European Physical Journal D</i> , 2014, 68, 1.	0.6	3
6748	Terahertz Vibrational Modes of the Rigid Crystal Phase of Succinonitrile. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2442-2446.	1.1	20
6749	Assessing the Performance of CASPT2 and DFT Methods for the Description of Long, Multicenter Bonding in Dimers between Radical Ions. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 650-658.	2.3	29
6750	Topology of the Interactions Pattern in Pharmaceutically Relevant Polymorphs of Methylxanthines (Caffeine, Theobromine, and Theophiline): Combined Experimental (¹ H- ¹⁴ N) Tj ETQq0,0,0 rgBT /Overlock 17 of Chemical Information and Modeling, 2014, 54, 2570-2584.	2.5	17
6751	A density functional study of chiral phosphoric acid-catalyzed direct arylation of trifluoromethyl ketone and diarylation of methyl ketone: reaction mechanism and the important role of the CF ₃ group. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 1908.	1.5	30
6752	Coordination of Halide and Chalcogenolate Anions to Heavier 1,2,5-Chalcogenadiazoles: Experiment and Theory. <i>Organometallics</i> , 2014, 33, 4302-4314.	1.1	60
6753	Heteroatom-Connected Ferrocenyl BODIPYs: Synthesis, Structure, and Properties. <i>Organometallics</i> , 2014, 33, 1867-1877.	1.1	40
6754	The origin of exo-stereoselectivity of norbornene in hetero Diels-Alder reactions. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 8079-8086.	1.5	14
6755	Radical Model of Arsenic(III) Toxicity: Theoretical and EPR Spin Trapping Studies. <i>Chemical Research in Toxicology</i> , 2014, 27, 765-774.	1.7	30
6756	Complex Mechanism of Relaxation in Solid Chloroxylenol (Antibacterial/Antifungal Agent) Studied by ¹ H NMR Spectroscopy and Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2209-2219.	1.1	7
6757	Evidence for Substrate Binding-Induced Zwitterion Formation in the Catalytic Cys-His Dyad of the SARS-CoV Main Protease. <i>Biochemistry</i> , 2014, 53, 5930-5946.	1.2	78

#	ARTICLE	IF	CITATIONS
6758	Versatile reactivity of Pd-catalysts: mechanistic features of the mono-N-protected amino acid ligand and cesium-halide base in Pd-catalyzed C-H bond functionalization. <i>Chemical Society Reviews</i> , 2014, 43, 5009-5031.	18.7	148
6759	A Strong Metal-to-Metal Interaction in an Edge-Sharing Biocubane Compound that Leads to a Very Short Tungsten-Tungsten Double Bond. <i>Inorganic Chemistry</i> , 2014, 53, 2288-2295.	1.9	10
6760	Theoretical study of linker-type effect in carbazole-carbazole-based dyes on performances of dye-sensitized solar cells. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	14
6761	The reaction mechanism of UDP-GlcNAc 5,6-dehydratase: a quantum mechanical/molecular mechanical (QM/MM) study. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	1
6762	Investigation of the torsional barrier of EDOT using molecular mechanics and DFT methods. <i>Journal of Molecular Modeling</i> , 2014, 20, 2405.	0.8	2
6763	Evidence of a long C-C attractive interaction in cerussite mineral: QTAIM and ELF analyses. <i>Journal of Molecular Modeling</i> , 2014, 20, 2425.	0.8	8
6764	Rational design of carbonitrile-carboxaldehyde cation receptor models: probing the nature of the heteroatom-metal interaction. <i>Journal of Molecular Modeling</i> , 2014, 20, 2428.	0.8	2
6765	Double coned inverse sandwich complexes $[M-(\eta^4-C_4H_4)-M]^{2+}$ of Gr-IA and Gr-IIA Metals: theoretical study of electronic of structure and second hyperpolarizability. <i>Journal of Molecular Modeling</i> , 2014, 20, 2440.	0.8	18
6766	The origin of exo-selectivity in methyl cyanofornate addition onto the C=C bond of norbornene in Pd-catalyzed cyanoesterification. <i>Dalton Transactions</i> , 2014, 43, 9537-9548.	1.6	11
6767	Noble-metal-free BODIPY-cobaloxime photocatalysts for visible-light-driven hydrogen production. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23884-23894.	1.3	50
6768	Investigation of transannular cycloaddition reactions involving furanoxonium ions using DFT calculations. Implications for the origin of plumarellide and rameswaralide and related polycyclic metabolites isolated from corals. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 7270-7278.	1.5	11
6769	Electron Transfer Initiated Formation of Covalently Bound Organic Layers on Silicon Surfaces. <i>Journal of Physical Chemistry C</i> , 2014, 118, 20908-20915.	1.5	5
6770	Fractional Charge Behavior and Band Gap Predictions with the XYG3 Type of Doubly Hybrid Density Functionals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9201-9211.	1.1	45
6771	Combined 3D-QSAR, molecular docking, and molecular dynamics study on potent cyclohexene-based influenza neuraminidase inhibitors. <i>Monatshefte für Chemie</i> , 2014, 145, 1213-1225.	0.9	11
6772	Synthesis, characterization, and evaluation of cis-diphenyl pyridineamine platinum(II) complexes as potential anti-breast cancer agents. <i>Journal of Biological Inorganic Chemistry</i> , 2014, 19, 967-979.	1.1	9
6773	First-principles study of Carbz-PAHTDDT dye sensitizer and two Carbz-derived dyes for dye sensitized solar cells. <i>Journal of Molecular Modeling</i> , 2014, 20, 2177.	0.8	17
6774	Sensitivity of ^3He NMR Parameters to the Proximity of Heterocyclic Rings. The Helium-Furan Dimer. <i>Chemistry of Heterocyclic Compounds</i> , 2014, 50, 421-428.	0.6	2
6775	Sensitivity of Noble Gas NMR Parameters to the Heterocyclic Ring Proximity. Density Functional Theory Studies of Ne-Furan and Ar-Furan Complexes. <i>Chemistry of Heterocyclic Compounds</i> , 2014, 50, 429-437.	0.6	4

#	ARTICLE	IF	CITATIONS
6776	Theoretical studies on effective metal-to-ligand charge transfer characteristics of novel ruthenium dyes for dye sensitized solar cells. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 565-575.	1.3	5
6777	Molecular insight of isotypes specific $\hat{\nu}^2$ -tubulin interaction of tubulin heterodimer with noscapinoids. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 751-763.	1.3	32
6778	Fluorescent Coumarin Derivatives with Viscosity Sensitive Emission - Synthesis, Photophysical Properties and Computational Studies. <i>Journal of Fluorescence</i> , 2014, 24, 1263-1274.	1.3	14
6779	Cyclic Azacyanines: Experimental and Computational Studies on Spectroscopic Properties and Unique Reactivity. <i>Journal of Fluorescence</i> , 2014, 24, 1285-1296.	1.3	2
6780	The Infrared Characterization and Mechanism of Oxygen Adsorption in Coal. <i>Spectroscopy Letters</i> , 2014, 47, 664-675.	0.5	58
6781	Direct observation of two-electron Ag(I)/Ag(III) redox cycles in coupling catalysis. <i>Nature Communications</i> , 2014, 5, 4373.	5.8	65
6782	Synthesis, Chiral Resolution, and Absolute Configuration of Dissymmetric 4,15-Difunctionalized [2.2]Paracyclophanes. <i>Journal of Organic Chemistry</i> , 2014, 79, 6679-6687.	1.7	33
6783	Theoretical Study of the Water Oxidation Mechanism with Non-heme Fe(Pytacn) Iron Complexes. Evidence That the Fe ^{IV} (O)(Pytacn) Species Cannot React with the Water Molecule To Form the O=O Bond. <i>Inorganic Chemistry</i> , 2014, 53, 5474-5485.	1.9	40
6784	Structural characterization, absorption and photoluminescence study of symmetrical azomethines with long aliphatic chains. <i>Journal of Molecular Structure</i> , 2014, 1058, 130-135.	1.8	26
6785	Electronic and Optical Structure of Wurtzite CuInS ₂ . <i>Journal of Physical Chemistry C</i> , 2014, 118, 14478-14484.	1.5	49
6786	General Multiobjective Force Field Optimization Framework, with Application to Reactive Force Fields for Silicon Carbide. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1426-1439.	2.3	107
6787	7-Azaindol-1-yl(organo)silanes and Their PdCl ₂ Complexes: Pd-Capped Tetrahedral Silicon Coordination Spheres and Paddlewheels with a Pd-Si Axis. <i>Organometallics</i> , 2014, 33, 2479-2488.	1.1	19
6788	Two hexaazatriphenylene based selective off-on fluorescent chemsensors for cadmium(II). <i>Talanta</i> , 2014, 119, 632-638.	2.9	16
6789	A review of the effect of multiple conformers on crystallization from solution and strategies for crystallizing slow inter-converting conformers. <i>Chemical Engineering Science</i> , 2014, 106, 275-292.	1.9	37
6790	Current-voltage characteristics through dithienylcyclopentene: A NEGF-DFT study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2014, 61, 1-8.	1.3	6
6791	Unrestricted density functional theory based on the fragment molecular orbital method for the ground and excited state calculations of large systems. <i>Journal of Chemical Physics</i> , 2014, 140, 144101.	1.2	19
6792	Unraveling the Mechanism of Water Oxidation Catalyzed by Nonheme Iron Complexes. <i>Chemistry - A European Journal</i> , 2014, 20, 5696-5707.	1.7	75
6793	Use of density functional theory in drug metabolism studies. <i>Expert Opinion on Drug Metabolism and Toxicology</i> , 2014, 10, 215-227.	1.5	25

#	ARTICLE	IF	CITATIONS
6794	Carbazole-BODIPY conjugates: design, synthesis, structure and properties. Dalton Transactions, 2014, 43, 13076.	1.6	50
6795	Density Functional Theory Calculations on the Complexation of <i>p</i> -Arsanilic Acid with Hydrated Iron Oxide Clusters: Structures, Reaction Energies, and Transition States. Journal of Physical Chemistry A, 2014, 118, 5667-5679.	1.1	28
6796	Selective Synthesis and Redox Sequence of a Heterobimetallic Nickel/Copper Complex of the Noninnocent Siamese-Twin Porphyrin. Inorganic Chemistry, 2014, 53, 7876-7885.	1.9	25
6797	Electronic Structures of Platinum(II) Complexes with 2-Arylpyridine and 1,3-Diketone Ligands: A Relativistic Density Functional Study on Photoexcitation and Phosphorescent Properties. Journal of Physical Chemistry C, 2014, 118, 12443-12449.	1.5	10
6798	The potential energy surface of singlet cyclobutadiene and substituted analogs: a coupled-cluster study. Structural Chemistry, 2014, 25, 635-648.	1.0	4
6799	Structure, tautomerism, and features of 1-(5-acetyl-2,4-dihydroxyphenyl)-3-(furan-2-yl)prop-2-en-1-one (FC) and 1,1- ϵ^2 -(4,6-dihydroxybenzene-1,3-diyl)bis[3-(furan-2-yl)prop-2-en-1-one] (FDC). Structural Chemistry, 2014, 25, 969-977.	1.0	4
6800	Direct ab initio dynamics calculations of thermal rate constants for the CH ₄ +O ₂ =CH ₃ +HO ₂ reaction. Structural Chemistry, 2014, 25, 1495-1503.	1.0	57
6801	Wavefunction and reactivity study of benzo[a]pyrene diol epoxide and its enantiomeric forms. Structural Chemistry, 2014, 25, 1521-1533.	1.0	370
6802	Sonochemical degradation of diclofenac: byproduct assessment, reaction mechanisms and environmental considerations. Environmental Science and Pollution Research, 2014, 21, 5929-5939.	2.7	37
6803	Quantum entanglement in photoactive prebiotic systems. Systems and Synthetic Biology, 2014, 8, 117-140.	1.0	14
6804	Second harmonic generation and electro-optical Pockels effect of 1- and 3-nitro-6-azabenz[a]pyrene N-oxide isomers: A Hartree-Fock and Coulomb-attenuating density functional theory investigation. Journal of Chemical Sciences, 2014, 126, 701-710.	0.7	2
6805	Computational mechanistic investigation of the gas phase C ₂ H ₄ +CO reaction on the singlet and triplet potential energy surfaces. Journal of the Iranian Chemical Society, 2014, 11, 781-790.	1.2	1
6806	A study of the role played by the Hartree-Fock orbital exchange in the formation of the energy of the first singlet charge-transfer excited state by the example of JK-62 and JK-201 sensitizing dye molecules. Optics and Spectroscopy (English Translation of Optika i Spektroskopiya), 2014, 116, 431-437.	0.2	4
6807	Reaction of CH ₃ CHO with Y ⁺ : A density functional theoretical study. Russian Journal of Physical Chemistry A, 2014, 88, 1158-1165.	0.1	1
6808	Photoinduced Proton Transfer and Isomerization in a Hydrogen-Bonded Aromatic Azo Compound: A CASPT2//CASSCF Study. Journal of Physical Chemistry A, 2014, 118, 4732-4739.	1.1	38
6809	From iridoids to dyes: a theoretical study on genipin reactivity. RSC Advances, 2014, 4, 11029.	1.7	13
6810	Quantitatively Probing the Al Distribution in Zeolites. Journal of the American Chemical Society, 2014, 136, 8296-8306.	6.6	199
6811	Surface properties of uranium dioxide from first principles. Journal of Nuclear Materials, 2014, 452, 479-485.	1.3	10

#	ARTICLE	IF	CITATIONS
6812	Density Functional Theoretical Modeling, Electrostatic Surface Potential and Surface Enhanced Raman Spectroscopic Studies on Biosynthesized Silver Nanoparticles: Observation of 400 pM Sensitivity to Explosives. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2904-2914.	1.1	29
6813	The Reverse Fluorine Perlin-like Effect and Related Stereoelectronic Interactions. <i>Journal of Organic Chemistry</i> , 2014, 79, 6385-6388.	1.7	19
6814	Molecular structure and stability of dissolved lithium polysulfide species. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10923-10932.	1.3	210
6815	(Photo)physical Properties of New Molecular Glasses End-Capped with Thiophene Rings Composed of Diimide and Imine Units. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13070-13086.	1.5	39
6816	Dynamic Effects on the Charge Transport in an Organic Near-Infrared Absorber Material. <i>Journal of Physical Chemistry C</i> , 2014, 118, 6537-6547.	1.5	15
6817	Nitroxidation of H-Terminated Si(111) Surfaces with Nitrobenzene and Nitrosobenzene. <i>Journal of Physical Chemistry C</i> , 2014, 118, 502-512.	1.5	29
6818	Ab initio studies on the proton dissociation and infrared spectra of sulfonated poly(ether ether) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 50	1.3	20
6819	Correlated Ab Initio and Density Functional Studies on H ₂ Activation by FeO ⁺ . <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3807-3820.	2.3	95
6820	Computational Evidence for the Detoxifying Mechanism of Epsilon Class Glutathione Transferase Toward the Insecticide DDT. <i>Environmental Science & Technology</i> , 2014, 48, 5008-5016.	4.6	47
6821	Mechanism of the Photoinduced Uncaging Reaction of Puromycin Protected by a 6-Nitroveratryloxycarbonyl Group. <i>Journal of the American Chemical Society</i> , 2014, 136, 3430-3438.	6.6	20
6822	A computational and experimental study of O-glycosylation. Catalysis by human UDP-GalNAc polypeptide:GalNAc transferase-T2. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 2645-2655.	1.5	39
6823	Polarizable Six-Point Water Models from Computational and Empirical Optimization. <i>Journal of Physical Chemistry B</i> , 2014, 118, 1589-1602.	1.2	24
6824	The average local ionization energy and Fukui function of l-ascorbate, the local reactivity descriptors of antioxidant reactivity. <i>Computational and Theoretical Chemistry</i> , 2014, 1049, 1-6.	1.1	17
6825	Seeking potential anticonvulsant agents that target GABAA receptors using experimental and theoretical procedures. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 1217-1232.	1.3	6
6826	Computational study on redox-switchable second-order nonlinear optical properties of ferrocene-tetrathiafulvalene hybrid. <i>RSC Advances</i> , 2014, 4, 38300-38309.	1.7	9
6827	Performance of DFT methods and origin of stereoselectivity in bipyridine N,N ⁺ -dioxide catalyzed allylation and propargylation reactions. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 8346-8353.	1.5	18
6828	Differential Control of Heme Reactivity in Alpha and Beta Subunits of Hemoglobin: A Combined Raman Spectroscopic and Computational Study. <i>Journal of the American Chemical Society</i> , 2014, 136, 10325-10339.	6.6	34
6829	Restricted Puckering of Mineralized RNA-Like Riboses. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5075-5081.	1.2	5

#	ARTICLE	IF	CITATIONS
6830	Atmospheric formation of the NO ₃ radical from gas-phase reaction of HNO ₃ acid with the NH ₂ radical: proton-coupled electron-transfer versus hydrogen atom transfer mechanisms. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19437-19445.	1.3	17
6831	Origins of Diastereoselectivity in Lewis Acid Promoted Ketene-Alkene [2 + 2] Cycloadditions. <i>Organic Letters</i> , 2014, 16, 5168-5171.	2.4	28
6832	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part I: Gas Phase. <i>ChemPhysChem</i> , 2014, 15, 3236-3245.	1.0	16
6833	Structure of the Catalytic Active Sites in Vanadium-Doped Aluminophosphate Microporous Materials. New Evidence from Spin Density Studies. <i>Journal of Physical Chemistry C</i> , 2014, 118, 19879-19888.	1.5	22
6834	Novel [2 + 1] Concerted Reaction Path for Disilacyclobutenes with Acetylene. <i>Organometallics</i> , 2014, 33, 763-770.	1.1	5
6835	Simulating Gold's Structure-Dependent Reactivity: Nonlocal Density Functional Theory Studies of Hydrogen Activation by Gold Clusters, Nanowires, and Surfaces. <i>Journal of Physical Chemistry C</i> , 2014, 118, 15693-15704.	1.5	9
6836	DFT investigation on structural stability, electronic properties and CO adsorption characteristics on anatase and rutile TiO ₂ nanostructures. <i>Ceramics International</i> , 2014, 40, 16147-16158.	2.3	17
6837	Polymorphism in Paracetamol: Evidence of Additional Forms IV and V at High Pressure. <i>Journal of Physical Chemistry A</i> , 2014, 118, 6068-6077.	1.1	31
6838	Implementation of nuclear gradients of range-separated hybrid density functionals and benchmarking on rotational constants for organic molecules. <i>Journal of Computational Chemistry</i> , 2014, 35, 1509-1516.	1.5	48
6839	Theoretical design of porphyrazine derivatives as promising sensitizers for dye-sensitized solar cells. <i>RSC Advances</i> , 2014, 4, 20200.	1.7	27
6840	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3151-3162.	2.3	23
6841	Towards a better understanding of magnetic exchange mediated by hydrogen bonds in Mn(III)/Fe(III) salen-type supramolecular dimers. <i>Dalton Transactions</i> , 2014, 43, 15602-15616.	1.6	39
6842	Poly(mono-, bi- or trifuran): effect of oligomer chain length on the electropolymerization performances and polymer properties. <i>RSC Advances</i> , 2014, 4, 14001-14012.	1.7	32
6843	Structures of Protonated Thymine and Uracil and Their Monohydrated Gas-Phase Ions from Ultraviolet Action Spectroscopy and Theory. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4256-4265.	1.1	32
6844	Accurate calculations of geometries and singlet-triplet energy differences for active-site models of [NiFe] hydrogenase. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7927-7938.	1.3	58
6845	Multi-intermediate-band character of Ti-substitutedCuGaS ₂ : Implications for photovoltaic applications. <i>Physical Review B</i> , 2014, 90, .	1.1	24
6846	Constrained Bithiazoles: Small Molecule Correctors of Defective F508-CFTR Protein Trafficking. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 6729-6738.	2.9	20
6847	Computed Propagation and Termination Steps in [(Cycloocta-2,6-dien-1-yl)RhIII(polymeryl)] ⁺ Catalyzed Carbene Polymerization Reactions. <i>ACS Catalysis</i> , 2014, 4, 1376-1389.	5.5	25

#	ARTICLE	IF	CITATIONS
6848	Electronic and Optical Properties of Dye-Sensitized TiO ₂ Interfaces. <i>Topics in Current Chemistry</i> , 2014, 347, 1-45.	4.0	18
6849	1,3- β -Silyl-elimination in electron-deficient cationic systems. <i>Chemical Science</i> , 2014, 5, 3983.	3.7	20
6850	π - π^* and σ - π conjugation, which is more efficient for intermolecular charge transfer in starburst triarylamine donors of platinum acetylide sensitizers?. <i>Dyes and Pigments</i> , 2014, 111, 21-29.	2.0	10
6851	Hybrid functionals applied to perovskites. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 253202.	0.7	81
6852	Influence of Donor Configurations on Photophysical, Electrochemical, and Photovoltaic Performances in D π A Organic Sensitizers. <i>ACS Sustainable Chemistry and Engineering</i> , 2014, 2, 239-247.	3.2	24
6853	Solvent-Dependent Decarboxylation of 1,3-Dimethylimidazolium-2-Carboxylate. <i>Journal of Organic Chemistry</i> , 2014, 79, 4293-4299.	1.7	37
6854	Electron Localization Function Study on the Chemical Bonding in a Real Space for Tetrahedrane, Cubane, Adamantane, and Dodecahedrane and Their Perfluorinated Derivatives and Radical Anions. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4147-4156.	1.1	15
6855	Monoanchoring (D π A) and Dianchoring (D π A) ₂ Organic Dyes Featuring Triarylamine Donors Composed of Fluorene and Carbazole. <i>Asian Journal of Organic Chemistry</i> , 2014, 3, 886-898.	1.3	8
6856	Assigning the EPR Fine Structure Parameters of the Mn(II) Centers in <i>Bacillus subtilis</i> Oxalate Decarboxylase by Site-Directed Mutagenesis and DFT/MM Calculations. <i>Journal of the American Chemical Society</i> , 2014, 136, 2313-2323.	6.6	17
6857	Structural, torsional, vibrational and response electric properties of 2,2-bitellurophene rotamers. An ab initio and density functional theory investigation. <i>Structural Chemistry</i> , 2014, 25, 959-968.	1.0	4
6858	Computational Study of the Kinetics and Mechanisms for the HCO + O ₃ Reaction. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3395-3401.	1.1	2
6859	Theoretical Design of n-Type Organic Semiconducting Materials Containing Thiazole and Oxazole Frameworks. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3335-3343.	1.1	32
6860	Pu@C ₂₄ : A New Example Satisfying the 32-Electron Principle. <i>Journal of Physical Chemistry C</i> , 2014, 118, 7211-7221.	1.5	26
6861	Thermochemical Properties and Bond Dissociation Enthalpies of 3- to 5-Member Ring Cyclic Ether Hydroperoxides, Alcohols, and Peroxy Radicals: Cyclic Ether Radical + 3O ₂ Reaction Thermochemistry. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3147-3167.	1.1	20
6862	Lanthanide and transition metal complexes of bioactive coumarins: Molecular modeling and spectroscopic studies. <i>Journal of Inorganic Biochemistry</i> , 2014, 135, 100-112.	1.5	28
6863	Dioxygen activation at room temperature during controllable and highly efficient acetaldehyde-to-acetic acid oxidation using a simple iron(III)-acetonitrile complex. <i>Catalysis Today</i> , 2014, 233, 140-146.	2.2	5
6864	Ammonia and hydrazine synthesis from [N ₂ -W{(NHCH ₂ CH ₂) ₃ N}] and [AH] ⁺ [BH] ⁻ using Sivasankar catalytic cycle: DFT studies. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 73-78.	1.1	9
6865	Influence of push-pull group substitution patterns on excited state properties of donor-acceptor co-monomers and their trimers. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 202-211.	1.1	7

#	ARTICLE	IF	CITATIONS
6866	Scope of chemical fixation of carbon dioxide catalyzed by a bifunctional monomeric tungstate. <i>Catalysis Today</i> , 2014, 226, 160-166.	2.2	39
6867	Effect of indium precursor and ligand type on the structure, morphology and surface functionalization of InP nanocrystals prepared by gas-liquid approach. <i>Synthetic Metals</i> , 2014, 187, 94-101.	2.1	4
6868	Fluorescence of PRODAN in water: A computational QM/MM MD study. <i>Chemical Physics Letters</i> , 2014, 597, 57-62.	1.2	14
6869	Corrole dyes for dye-sensitized solar cells: The crucial role of the dye/semiconductor energy level alignment. <i>Computational and Theoretical Chemistry</i> , 2014, 1030, 59-66.	1.1	38
6870	Experimental and theoretical study of the mechanism of formation of astrochemically important $C_{2n+1}N^+$ anions via ion/molecule reactions. <i>International Journal of Mass Spectrometry</i> , 2014, 367, 1-9.	0.7	7
6871	Theoretical insight into the pyrolytic deformylation of levoglucosenone and isolevoglucosenone. <i>Carbohydrate Research</i> , 2014, 390, 76-80.	1.1	16
6872	Theoretical investigation on the chemo- and stereoselectivities of isoleucine-catalyzed cross-aldol reactions between two enolizable aldehydes involving isobutyraldehyde and contrasts with proline catalysis. <i>Tetrahedron: Asymmetry</i> , 2014, 25, 418-428.	1.8	2
6873	Hybrid density functional calculations of the defect properties of ZnO:Rh and ZnO:Ir. <i>Thin Solid Films</i> , 2014, 555, 112-116.	0.8	10
6874	Direct dynamics study on the reaction of 1,1-difluoroethane with hydrogen trioxide radical. <i>Computational and Theoretical Chemistry</i> , 2014, 1034, 53-60.	1.1	2
6875	Quantum chemical perspective of efficient NLO materials based on dipolar trans-tetraammineruthenium (II) complexes with pyridinium and thiocyanate ligands: First theoretical framework. <i>Computational and Theoretical Chemistry</i> , 2014, 1033, 6-13.	1.1	42
6876	On site coulomb repulsion dominates over the non-local Hartree-Fock exchange in determining the band gap of polymers. <i>Journal of Physics and Chemistry of Solids</i> , 2014, 75, 212-223.	1.9	4
6877	Theoretical constraints on the effects of pH, salinity, and temperature on clumped isotope signatures of dissolved inorganic carbon species and precipitating carbonate minerals. <i>Geochimica Et Cosmochimica Acta</i> , 2014, 125, 610-652.	1.6	123
6878	Stacking interactions of nickel bis(dithiolene) with benzene. <i>Chemical Physics Letters</i> , 2014, 591, 29-31.	1.2	1
6879	A comparative DFT study on the differences between normal modes of polyethylene and polyethylene glycol via B3LYP Hamiltonian and the Hartree-Fock method in multiple bases. <i>Optik</i> , 2014, 125, 228-231.	1.4	8
6880	A simplified time-dependent density functional theory approach for electronic ultraviolet and circular dichroism spectra of very large molecules. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 45-53.	1.1	211
6881	Multiscale Free Energy Simulations: An Efficient Method for Connecting Classical MD Simulations to QM or QM/MM Free Energies Using Non-Boltzmann Bennett Reweighting Schemes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1406-1419.	2.3	111
6882	Investigation of Thermochemistry Associated with the Carbon-Carbon Coupling Reactions of Furan and Furfural Using ab Initio Methods. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4392-4404.	1.1	6
6883	Identification and Characterization of Noncovalent Interactions That Drive Binding and Specificity in DD-Peptidases and β -Lactamases. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 855-864.	2.3	15

#	ARTICLE	IF	CITATIONS
6884	Predicting Solar-Cell Dyes for Cosensitization. <i>Journal of Physical Chemistry C</i> , 2014, 118, 14082-14090.	1.5	15
6885	Effect of the Meso-Substituent in the Hückel-to-Möbius Topological Switches. <i>Journal of Organic Chemistry</i> , 2014, 79, 5036-5046.	1.7	27
6886	A Mechanistic Study of the Lewis Base-Directed Cycloaddition of 2-Pyrones and Alkynylboranes. <i>Journal of the American Chemical Society</i> , 2014, 136, 8642-8653.	6.6	31
6887	Mechanisms and Origins of Switchable Regioselectivity of Palladium- and Nickel-Catalyzed Allene Hydrosilylation with N-Heterocyclic Carbene Ligands: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 4517-4527.	1.7	57
6888	Experimental and Computational Studies of the Neutral and Reduced States of Indeno[1,2- <i>b</i>]fluorene. <i>Journal of the American Chemical Society</i> , 2014, 136, 9181-9189.	6.6	41
6889	9,9- ϵ^2 -Spirofluorene and 4-phenyl-9,9- ϵ^2 -spirofluorene: pure hydrocarbon small molecules as hosts for efficient green and blue PhOLEDs. <i>Journal of Materials Chemistry C</i> , 2014, 2, 4156-4166.	2.7	75
6890	Exploring Water Catalysis in the Reaction of Thioformic Acid with Hydroxyl Radical: A Global Reaction Route Mapping Perspective. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4019-4029.	1.1	19
6891	Mechanism of Oxygen Exchange between CO ₂ and TiO ₂ (101) Anatase. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1628-1639.	1.5	31
6892	Organic Dyes Containing Fluorene Decorated with Imidazole Units for Dye-Sensitized Solar Cells. <i>Journal of Organic Chemistry</i> , 2014, 79, 3159-3172.	1.7	71
6893	Branching Out from the Bisaboly Cation. Unifying Mechanistic Pathways to Barbatene, Bazzanene, Chamigrene, Chamipinene, Cumacrene, Cuprenene, Dunniene, Isobazzanene, Iso- β^3 -bisabolene, Isochamigrene, Laurene, Microbiotene, Sesquithujene, Sesquisabinene, Thujopsene, Trichodiene, and Widdradiene Sesquiterpenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 2450-2463.	6.6	95
6894	Structural findings of quinolone carboxylic acids in cytotoxic, antiviral, and anti-HIV-1 integrase activity through validated comparative molecular modeling studies. <i>Medicinal Chemistry Research</i> , 2014, 23, 3096-3127.	1.1	18
6895	Dearomative Indole (3 + 2) Cycloaddition Reactions. <i>Journal of the American Chemical Society</i> , 2014, 136, 6288-6296.	6.6	141
6896	Mn K-Edge X-ray Absorption Studies of Oxo- and Hydroxo-manganese(IV) Complexes: Experimental and Theoretical Insights into Pre-Edge Properties. <i>Inorganic Chemistry</i> , 2014, 53, 6179-6194.	1.9	54
6897	2-Methyl-4-oxo-N-(4-oxo-2-phenyl) 1,3,4-dihydroquinolin-2(1H)-one (substituted-1,3-thiazolidin-3-yl)-3,4-dihydroquinolin-2(1H)-one Whitening Agents: Synthesis and Photophysical Characterization. <i>Journal of Fluorescence</i> , 2014, 24, 1077-1086.	1.3	16
6898	Tuning the Adsorption Interactions of Imidazole Derivatives with Specific Metal Cations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3944-3951.	1.1	14
6899	Disklike Hepta- and Tridecanuclear Cobalt Clusters. Synthesis, Structures, Magnetic Properties, and DFT Calculations. <i>Inorganic Chemistry</i> , 2014, 53, 5458-5466.	1.9	43
6900	Experimental and Theoretical Insights into the Mechanisms of Sulfate and Sulfamate Ester Hydrolysis and the End Products of Type I Sulfatase Inactivation by Aryl Sulfamates. <i>Journal of Organic Chemistry</i> , 2014, 79, 1995-2005.	1.7	32
6901	Organic dyes containing fluoren-9-ylidene chromophores for efficient dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2014, 2, 5766.	5.2	60

#	ARTICLE	IF	CITATIONS
6902	Designing Conical Intersections for Light-Driven Single Molecule Rotary Motors: From Precessional to Axial Motion. <i>Journal of Organic Chemistry</i> , 2014, 79, 3587-3600.	1.7	67
6903	Evaluation of various density functionals for predicting the electrophosphorescent host HOMO, LUMO and triplet energies. <i>Synthetic Metals</i> , 2014, 195, 54-60.	2.1	15
6904	trans -[Ru(NO)(NH ₃) ₃ P(O ⁺)(OEt) ₂] ²⁺ : A new and robust NO/HNO-donor in aqueous media. <i>Inorganica Chimica Acta</i> , 2014, 421, 74-79.	1.2	13
6905	Quantum Mechanics/Molecular Mechanics Study of Oxygen Binding in Hemocyanin. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5034-5043.	1.2	18
6906	Applications of Time Dependent and Time Independent Density Functional Theory to the First $\tilde{\text{I}}\epsilon$ to $\tilde{\text{I}}\epsilon^*$ Transition in Cyanine Dyes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3299-3307.	2.3	79
6907	Investigation of the reactions of U, U ⁺ and U ²⁺ with ammonia: mechanisms and topological analysis. <i>RSC Advances</i> , 2014, 4, 29806.	1.7	20
6908	First Principles LDA+U Calculations for ZnO Materials. <i>Integrated Ferroelectrics</i> , 2014, 155, 15-22.	0.3	71
6909	Design and synthesis of novel active phosphonate esters and their application in preparation of ceftriaxone. <i>Heterocyclic Communications</i> , 2014, 20, 155-159.	0.6	3
6910	Generalized Energy-Based Fragmentation CCSD(T)-F12a Method and Application to the Relative Energies of Water Clusters (H ₂ O) ₂₀ . <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1546-1553.	2.3	62
6911	A QSPR approach for the fast estimation of DFT/NBO partial atomic charges. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2014, 134, 158-163.	1.8	20
6912	Synthesis, structure, spectral, thermal analyses and DFT calculation of a hydrogen bonded crystal: 2-Aminopyrimidinium dihydrogenphosphate monohydrate. <i>Journal of Molecular Structure</i> , 2014, 1074, 107-117.	1.8	20
6913	Studies on molecular structure, vibrational spectra and molecular docking analysis of 3-Methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl 4-aminobenzoate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 130, 591-603.	2.0	9
6914	Exploring the Conical Intersection Seam in Cytosine: A DFT and CASSCF Study. <i>Procedia Computer Science</i> , 2014, 29, 1384-1391.	1.2	1
6915	Monothioanthraquinone as an organic active material for greener lithium batteries. <i>Journal of Power Sources</i> , 2014, 267, 553-559.	4.0	56
6916	Theoretical study on the mechanism and thermodynamic of methanethiol and ozone reaction. <i>Computational and Theoretical Chemistry</i> , 2014, 1042, 41-48.	1.1	3
6917	2-Substituted vs 4-substituted-9,9 ϵ^2 -spirobifluorene host materials for green and blue phosphorescent OLEDs: a structure ϵ^2 property relationship study. <i>Tetrahedron</i> , 2014, 70, 6337-6351.	1.0	43
6918	TABS: A database of molecular structures. <i>Computational and Theoretical Chemistry</i> , 2014, 1043, 13-16.	1.1	21
6919	A comprehensive spectroscopic and computational investigation of intramolecular proton transfer in the excited states of 2-(2 ϵ^2 -hydroxyphenyl) benzoxazole and its derivatives. <i>Journal of Luminescence</i> , 2014, 146, 527-538.	1.5	38

#	ARTICLE	IF	CITATIONS
6960	Crystal structure optimisation using an auxiliary equation of state. <i>Journal of Chemical Physics</i> , 2015, 143, 184101.	1.2	21
6961	Fast, accurate evaluation of exact exchange: The occ-RI-K algorithm. <i>Journal of Chemical Physics</i> , 2015, 143, 024113.	1.2	44
6962	Fermi orbital self-interaction corrected electronic structure of molecules beyond local density approximation. <i>Journal of Chemical Physics</i> , 2015, 143, 224104.	1.2	29
6963	Computational Prediction of One-Step Synthesis of Seven-membered Fused Rings by (5+2) Cycloaddition Utilising Cycloalkenes. <i>Scientific Reports</i> , 2015, 5, 12272.	1.6	2
6964	Response to "Comment on "Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0" [J. Chem. Phys. 143, 187101 (2015)]. <i>Journal of Chemical Physics</i> , 2015, 143, 187102.	1.2	8
6965	Charge-ordering induces magnetic axes rotation in organic materials (TMTTF) ₂ X (with X = SbF ₆ , AsF ₆). <i>Tj ETQq1 1 0.784314 JgBT /Over</i>	0.2	0
6966	Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. <i>Journal of Chemical Physics</i> , 2015, 143, 134702.	1.2	84
6967	Exciton size and binding energy limitations in one-dimensional organic materials. <i>Journal of Chemical Physics</i> , 2015, 143, 244905.	1.2	59
6968	Quantum Monte Carlo calculation of the binding energy of the beryllium dimer. <i>Journal of Chemical Physics</i> , 2015, 143, 084116.	1.2	26
6969	Photodissociation dynamics of CH ₃ C(O)SH in argon matrix: A QM/MM nonadiabatic dynamics simulation. <i>Journal of Chemical Physics</i> , 2015, 143, 194303.	1.2	12
6970	Computational discovery of lanthanide doped and Co-doped Y ₃ Al ₅ O ₁₂ for optoelectronic applications. <i>Applied Physics Letters</i> , 2015, 107, 112109.	1.5	10
6971	A novel Gaussian-Sinc mixed basis set for electronic structure calculations. <i>Journal of Chemical Physics</i> , 2015, 143, 064108.	1.2	11
6972	Singles correlation energy contributions in solids. <i>Journal of Chemical Physics</i> , 2015, 143, 102816.	1.2	39
6973	A self-consistent first-principle based approach to model carrier mobility in organic materials. <i>AIP Conference Proceedings</i> , 2015, , .	0.3	0
6974	Effect of ensemble generalization on the highest-occupied Kohn-Sham eigenvalue. <i>Journal of Chemical Physics</i> , 2015, 143, 104105.	1.2	16
6975	Construction of exchange-correlation functionals through interpolation between the non-interacting and the strong-correlation limit. <i>Journal of Chemical Physics</i> , 2015, 143, 124103.	1.2	23
6976	Calculation of the spectrum of quasiparticle electron excitations in organic molecular semiconductors. <i>Journal of Experimental and Theoretical Physics</i> , 2015, 120, 1093-1100.	0.2	1
6977	Communication: Hole localization in Al-doped quartz SiO ₂ within <i>ab initio</i> hybrid-functional DFT. <i>Journal of Chemical Physics</i> , 2015, 143, 111103.	1.2	32

#	ARTICLE	IF	CITATIONS
6978	Orbitals with intermediate localization and low coupling: Spanning the gap between canonical and localized orbitals. <i>Journal of Chemical Physics</i> , 2015, 143, 014106.	1.2	8
6979	A DFT Study on the Dissociation Property of Sulfonic Acids with Different Neighboring Pendants in Polymer Electrolyte Membranes. , 2015, , .		0
6980	Environmental effects on Cu(II)-catalyzed hetero-Diels-Alder reactions: computational approach. <i>Monatshefte für Chemie</i> , 2015, 146, 1267-1274.	0.9	0
6981	Breathing Raman modes in Ag ₂ S nanoparticles obtained from F9 zeolite matrix. <i>Chemical Physics</i> , 2015, 463, 106-110.	0.9	15
6982	Quasiparticle band structure. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2015, 200, 181-192.	0.8	2
6983	A first-principles study of chlorine adsorption characteristics on \pm -Cr ₂ O ₃ nanostructures. <i>Journal of Chemical Sciences</i> , 2015, 127, 1785-1794.	0.7	6
6984	Near-UV photodissociation of phosphopeptide cation-radicals. <i>International Journal of Mass Spectrometry</i> , 2015, 390, 71-80.	0.7	9
6985	Thermal formation of hydroxynitriles, precursors of hydroxyacids in astrophysical ice analogs: Acetone ((CH ₃) ₂ CO) and hydrogen cyanide (HCN) reactivity. <i>Molecular Astrophysics</i> , 2015, 1, 1-12.	1.7	3
6986	Theoretical Studies of the Reactions CF ₃ H ₃ ⁺ COOR+Cl and CF ₃ COOCH ₃ +OH. <i>ChemPhysChem</i> , 2015, 16, 1768-1776.	1.0	16
6987	A Computational Comparison of Oxygen Atom Transfer Catalyzed by Dimethyl Sulfoxide Reductase with Mo and W. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 3580-3589.	1.0	23
6988	Hydroxylamine synthesis by oxygen insertion into Re ξ ;NH ₂ bond via Baeyer-Villiger oxidation: a Theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 690-694.	0.9	0
6989	N-doped Carbon Networks: Alternative Materials Tracing New Routes for Activating Molecular Hydrogen. <i>Chemistry - A European Journal</i> , 2015, 21, 3806-3814.	1.7	11
6990	Unraveling the Electronic Structure, Spin States, Optical and Vibrational Spectra of Malaria Pigment. <i>Chemistry - A European Journal</i> , 2015, 21, 8544-8553.	1.7	5
6991	Rh ^{III} -Catalyzed C(sp ³) ₃ H Bond Activation by an External Base Metalation/Deprotonation Mechanism: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2015, 21, 11158-11164.	1.7	38
6992	Core Halogenation as a Construction Principle in Tuning the Material Properties of Tetraazaperopyrenes. <i>Chemistry - A European Journal</i> , 2015, 21, 17691-17700.	1.7	35
6993	Efficient Rhodium-Catalyzed Multicomponent Reaction for the Synthesis of Novel Propargylamines. <i>Chemistry - A European Journal</i> , 2015, 21, 17701-17707.	1.7	27
6994	Molecular Engineering of Pyrido[3,4-b]pyrazine-Based Donor-Acceptor-Acceptor Organic Sensitizers: Effect of Auxiliary Acceptor in Cobalt- and Iodine-Based Electrolytes. <i>Chemistry - A European Journal</i> , 2015, 21, 18654-18661.	1.7	13
6995	Indaphyrins and Indachlorins: Optical and Chiroptical Properties of a Family of Helimeric Porphyrinoids. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 3913-3922.	1.2	24

#	ARTICLE	IF	CITATIONS
6996	Thieno[3,2- <i>b</i>][1]benzothiophene Derivative as a New Bridge Unit in Dye-Sensitized Solar Cells. <i>Advanced Energy Materials</i> , 2015, 5, 1500300.	10.2	138
6997	<i>meso</i> -Aryl [28]Hexaphyrin Silicon Complexes Bearing Various <i>Si</i> -Substituents and 1,16-Dihydrohexaphyrin bis-Chlorosilicon Complex. <i>Chemistry - an Asian Journal</i> , 2015, 10, 2200-2206.	1.7	14
6998	Reactivity of a Nickel(II) Bis(amidate) Complex with <i>meta</i> -Chloroperbenzoic Acid: Formation of a Potent Oxidizing Species. <i>Chemistry - A European Journal</i> , 2015, 21, 15029-15038.	1.7	82
6999	Triphenylguanidine-Promoted ortho-Metalation Reaction in a Triply Bonded Dirhenium System - Spectroscopic, Structural, and Computational Studies. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 1759-1765.	1.0	4
7000	Probing the range of applicability of structure- and energy-adjusted QM/MM link bonds. <i>Journal of Computational Chemistry</i> , 2015, 36, 1929-1939.	1.5	17
7001	An ab initio Based Structure Property Relationship for Prediction of Ignition Delay of Hypergolic Ionic Liquids. <i>Propellants, Explosives, Pyrotechnics</i> , 2015, 40, 759-764.	1.0	14
7002	Effects of calcium complexation on heparin-like disaccharides. A combined theoretical, tandem mass spectrometry and ultraviolet experiment. <i>Rapid Communications in Mass Spectrometry</i> , 2015, 29, 1135-1144.	0.7	8
7003	Highly Antiplasmodial Non-Natural Oxidative Products of Dioncophylline...A: Synthesis, Absolute Configuration, and Conformational Stability. <i>Chemistry - A European Journal</i> , 2015, 21, 14507-14518.	1.7	11
7004	Elucidating collision induced dissociation products and reaction mechanisms of protonated uracil by coupling chemical dynamics simulations with tandem mass spectrometry experiments. <i>Journal of Mass Spectrometry</i> , 2015, 50, 1340-1351.	0.7	31
7005	A DFT study of hydride transfers to the carbonyl oxygen of DDQ. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1533-1542.	1.0	11
7006	Coordination-resolved bonding and electronic dynamics of Na atomic clusters and solid skins. <i>RSC Advances</i> , 2015, 5, 35274-35281.	1.7	9
7007	New density functional parameterizations to accurate calculations of electric field gradient variations among compounds. <i>Journal of Computational Chemistry</i> , 2015, 36, 2125-2130.	1.5	2
7008	Comparison of the Full Catalytic Cycle of Hydroformylation Mediated by Mono- and Bis-Ligated Triphenylphosphine-Rhodium Complexes by Using DFT Calculations. <i>ChemCatChem</i> , 2015, 7, 1708-1718.	1.8	35
7009	Total Synthesis of (\pm)-Hippolachnin...A. <i>Angewandte Chemie</i> , 2015, 127, 2408-2412.	1.6	21
7010	Ruthenium-Grafted Vinylhelicenes: Chiroptical Properties and Redox Switching. <i>Chemistry - A European Journal</i> , 2015, 21, 17100-17115.	1.7	43
7011	Enantioselective Preparation, Conformational Analysis and Absolute Configuration of Highly Substituted Aziridines. <i>Chirality</i> , 2015, 27, 875-887.	1.3	4
7012	Conformational Structures of a Decapeptide Validated by First Principles Calculations and Cold Ion Spectroscopy. <i>ChemPhysChem</i> , 2015, 16, 1374-1378.	1.0	28
7013	Solvent-Free Iridium-Catalyzed Reactivity of CO ₂ with Secondary Amines and Hydrosilanes. <i>ChemCatChem</i> , 2015, 7, 3895-3902.	1.8	40

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7014	Mapping the Interactions of I^{2+} , I^{+} , I^{\bullet} , and I^{+} with Alkynes and Their Roles in Iodocyclizations. <i>Chemistry - A European Journal</i> , 2015, 21, 10191-10199.	1.7	24
7015	Oligoene-Based π -Helicenes or Dispiranes? Winding up Oligoene Chains by a Multiple Carbopalladation/Stille/(Electrocyclization) Cascade. <i>Chemistry - A European Journal</i> , 2015, 21, 16136-16146.	1.7	22
7016	An Insight into Transfer Hydrogenation Reactions Catalysed by Iridium(III) Bis-N-heterocyclic Carbenes. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 4388-4395.	1.0	17
7017	Effects of the ionization in the tautomerism of uracil: A reaction electronic flux perspective. <i>Journal of Computational Chemistry</i> , 2015, 36, 2135-2145.	1.5	6
7018	Development of a sensitive, stable and EGFR-specific molecular imaging agent for surface enhanced Raman spectroscopy. <i>Journal of Raman Spectroscopy</i> , 2015, 46, 434-446.	1.2	22
7020	A Theoretical Study on Superexchange Interaction in KCoF_3 and $\text{Cs}_{1-x}\text{Na}_x\text{Mn}(\text{CN})_3$ by Chemical Bonding Rule. <i>Journal of Computer Chemistry Japan</i> , 2015, 13, 319-320.	0.0	2
7021	Trifluoromethyl-substituted tetrathiafulvalenes. <i>Beilstein Journal of Organic Chemistry</i> , 2015, 11, 647-658.	1.3	6
7022	Experimental and Theoretical Investigations on the Supramolecular Structure of Isoliquiritigenin and 6-O- β -D-Maltosyl- β -cyclodextrin Inclusion Complex. <i>International Journal of Molecular Sciences</i> , 2015, 16, 17999-18017.	1.8	26
7023	Assessing Covalency in Cerium and Uranium Hexachlorides: A Correlated Wavefunction and Density Functional Theory Study. <i>Inorganics</i> , 2015, 3, 482-499.	1.2	33
7024	Aqua-Vanadyl Ion Interaction with Nafion [®] Membranes. <i>Frontiers in Energy Research</i> , 2015, 3, .	1.2	7
7025	A New Index for the Estimation of the Aromatic Character - IX. <i>Letters in Organic Chemistry</i> , 2015, 13, 33-43.	0.2	5
7026	Asymmetric Total Synthesis of (β)-4-Hydroxyzinowol, a Highly Oxygenated Dihydro- β -Agarofuran. <i>Yuki Gosei Kagaku Kyokaiishi/Journal of Synthetic Organic Chemistry</i> , 2015, 73, 1081-1091.	0.0	2
7027	Elucidation of Enzymatic Mechanism of Phenazine Biosynthetic Protein PhzF Using QM/MM and MD Simulations. <i>PLoS ONE</i> , 2015, 10, e0139081.	1.1	6
7028	Charge carrier mobility and electronic properties of $\text{Al}(\text{Op})_3$: impact of excimer formation. <i>Beilstein Journal of Nanotechnology</i> , 2015, 6, 1107-1115.	1.5	7
7029	Chemical Empiricism 2.0 at Age of Big Data: Large-scale Prediction of Reaction Pathways Based on Bond Dissociation Energies. <i>Chinese Journal of Chemical Physics</i> , 2015, 28, 674-680.	0.6	0
7031	Homocoupling versus reduction of radicals: an experimental and theoretical study of $\text{Ti}(\text{scp})_3$ -mediated deoxygenation of activated alcohols. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 3462-3469.	1.5	26
7032	An experimental and theoretical study of the kinetics of the reaction between 3-hydroxy-3-methyl-2-butanone and OH radicals. <i>RSC Advances</i> , 2015, 5, 26559-26568.	1.7	12
7033	The relationship between the boron dipyromethene (BODIPY) structure and the effectiveness of homogeneous and heterogeneous solar hydrogen-generating systems as well as DSSCs. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9716-9729.	1.3	54

#	ARTICLE	IF	CITATIONS
7034	New thiocyanate-free ruthenium(II) sensitizers with different pyrid-2-yl tetrazolate ligands for dye-sensitized solar cells. <i>Dalton Transactions</i> , 2015, 44, 11788-11796.	1.6	28
7035	Effect of Hartree-Fock exact exchange on intramolecular magnetic coupling constants of organic diradicals. <i>Journal of Chemical Physics</i> , 2015, 142, 024318.	1.2	21
7036	Critical evaluation of the potential energy surface of the $\text{CH}_3 + \text{HO}_2$ reaction system. <i>Journal of Chemical Physics</i> , 2015, 142, 054308.	1.2	11
7037	Wide Band-Gap 3,4-Difluorothiophene-Based Polymer with 7% Solar Cell Efficiency: An Alternative to P3HT. <i>Chemistry of Materials</i> , 2015, 27, 4184-4187.	3.2	102
7038	Tuning Range-Separated Density Functional Theory for Photocatalytic Water Splitting Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1700-1709.	2.3	64
7039	Congeners of Pyromethene-567 Dye: Perspectives from Synthesis, Photophysics, Photostability, Laser, and TD-DFT Theory. <i>Journal of Organic Chemistry</i> , 2015, 80, 6152-6164.	1.7	59
7040	Mechanism and Stereoselectivity of Directed $\text{C}(\text{sp}^3)\text{-H}$ Activation and Arylation Catalyzed by Pd(II) with Pyridine Ligand and Trifluoroacetate: A Computational Study. <i>ACS Catalysis</i> , 2015, 5, 3648-3661.	5.5	29
7041	Global Hybrids from the Semiclassical Atom Theory Satisfying the Local Density Linear Response. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 122-131.	2.3	22
7042	Catalytic Mechanism of Cofactor-Free Dioxygenases and How They Circumvent Spin-Forbidden Oxygenation of Their Substrates. <i>Journal of the American Chemical Society</i> , 2015, 137, 7474-7487.	6.6	70
7043	Adsorption and sub-nanomolar sensing of thioflavin T on colloidal gold nanoparticles, silver nanoparticles and silver-coated films studied using surface-enhanced Raman scattering. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 149, 949-956.	2.0	22
7044	Unusual case of desmotropy. Combined spectroscopy (^1H - ^{14}N NQDR) and quantum chemistry (periodic) Tj ETQq0 0 0 rgBT /Overlock 1 State Nuclear Magnetic Resonance, 2015, 68-69, 13-24.	1.5	1
7045	Mechanistic Studies on the Alkylation of Amines with Alcohols Catalyzed by a Bifunctional Iridium Complex. <i>ACS Catalysis</i> , 2015, 5, 3704-3716.	5.5	72
7046	Metalloradical-Catalyzed Selective 1,2-Rh-H Insertion into the Aliphatic Carbon-Carbon Bond of Cyclooctane. <i>Organometallics</i> , 2015, 34, 2849-2857.	1.1	8
7047	Highly efficient conversion of CO_2 at atmospheric pressure to cyclic carbonates with in situ-generated homogeneous catalysts from a copper-containing coordination polymer. <i>Journal of Catalysis</i> , 2015, 329, 119-129.	3.1	65
7048	Methane adsorption characteristics on In^{2+} -Ga 2O_3 nanostructures: DFT investigation. <i>Applied Surface Science</i> , 2015, 344, 65-78.	3.1	16
7049	Computational Molecular Electronic Spectroscopy with TD-DFT. <i>Topics in Current Chemistry</i> , 2015, 368, 347-375.	4.0	29
7050	Many-Body Perturbation Theory (MBPT) and Time-Dependent Density-Functional Theory (TD-DFT): MBPT Insights About What Is Missing In, and Corrections To, the TD-DFT Adiabatic Approximation. <i>Topics in Current Chemistry</i> , 2015, 368, 1-60.	4.0	21
7051	Electric properties of the low-lying excited states of benzonitrile: geometry relaxation and solvent effects. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	13

#	ARTICLE	IF	CITATIONS
7052	Theoretical investigation of HNgNH ₃ ⁺ ions (Ng = He, Ne, Ar, Kr, and Xe). <i>Journal of Chemical Physics</i> , 2015, 142, 144301.	1.2	6
7053	Further insights into the structure and chemistry of the Gilsonite asphaltene from a combined theoretical and experimental approach. <i>Fuel</i> , 2015, 157, 16-20.	3.4	35
7054	Quantifying solvated electrons' delocalization. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 18305-18317.	1.3	22
7055	Role of exchange and correlation in the real external prediction of mutagenicity: performance of hybrid and meta-hybrid exchange–correlation functionals. <i>RSC Advances</i> , 2015, 5, 29238-29251.	1.7	17
7056	Inter molecular azide–diisocyanate coupling: new insights for energetic solid propellants. <i>RSC Advances</i> , 2015, 5, 50478-50482.	1.7	6
7057	Analytic second derivative of the energy for density functional theory based on the three-body fragment molecular orbital method. <i>Journal of Chemical Physics</i> , 2015, 142, 124101.	1.2	12
7058	Assessment of hybrid, meta-hybrid-GGA, and long-range corrected density functionals for the estimation of enthalpies of formation, barrier heights, and ionisation potentials of selected C1–C5 oxygenates. <i>Molecular Physics</i> , 2015, 113, 1630-1635.	0.8	8
7059	First-Principles Calculation of Phonon and Schottky Heat Capacities of Plutonium Dioxide. <i>Journal of the Physical Society of Japan</i> , 2015, 84, 053602.	0.7	4
7060	Structural findings of phenylindoles as cytotoxic antimetabolic agents in human breast cancer cell lines through multiple validated QSAR studies. <i>Toxicology in Vitro</i> , 2015, 29, 1392-1404.	1.1	32
7061	Mechanisms of σ -, π -, and δ -H(D) Exchange Processes in the σ -Agostic Alkyltitanocene(IV) Complexes [Cp ₂ TiCH ₂ CH(CH ₃)(CMe ₃)] ⁺ and [Cp ₂ TiCH ₂ CH(CD ₃)(CMe ₃)] ⁺ : Stark Contrasts with Their β -SiMe ₃ Analogues. <i>Organometallics</i> , 2015, 34, 2356-2368.	1.1	5
7062	NO adsorption studies on silicene nanosheet: DFT investigation. <i>Applied Surface Science</i> , 2015, 351, 662-672.	3.1	95
7063	Inquiry of the reaction paths in thermal retro-Diels–Alder reactions in the gas phase: Theoretical study on the concerted and stepwise elimination mechanisms of cyclohexenes. <i>Computational and Theoretical Chemistry</i> , 2015, 1067, 103-113.	1.1	3
7064	Photoinduced Ultrafast Intramolecular Excited-State Energy Transfer in the Silylene-Bridged Biphenyl and Stilbene (SBS) System: A Nonadiabatic Dynamics Point of View. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6937-6948.	1.1	10
7065	Photophysical and photosensitizing characters of 2-phenylbenzimidazole-5-sulfonic acid. A theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 187-189.	2.0	4
7066	In-situ Spectroscopic Investigation of the Rhenium–Catalyzed Deoxydehydration of Vicinal Diols. <i>ChemCatChem</i> , 2015, 7, 1184-1196.	1.8	21
7067	Reactivity Modes of an Iron Bis(alkoxide) Complex with Aryl Azides: Catalytic Nitrene Coupling vs Formation of Iron(III) Imido Dimers. <i>Organometallics</i> , 2015, 34, 2917-2923.	1.1	43
7068	Combining Near-UV Photodissociation with Electron Transfer. Reduction of the Diazirine Ring in a Photomethionine-Labeled Peptide Ion. <i>Journal of the American Society for Mass Spectrometry</i> , 2015, 26, 1367-1381.	1.2	10
7069	Coordination-resolved local bond strain and 3p energy entrapment of K atomic clusters and K(1 1 0) skin. <i>Applied Surface Science</i> , 2015, 349, 665-672.	3.1	0

#	ARTICLE	IF	CITATIONS
7070	Interaction between PH3 and small water clusters: Understanding the electronic and spectroscopic properties. Computational and Theoretical Chemistry, 2015, 1059, 35-44.	1.1	21
7071	The quest for energy traps in the CP43 antenna of photosystem II. Journal of Photochemistry and Photobiology B: Biology, 2015, 152, 286-300.	1.7	21
7072	Intramolecular fixation of t-butyl groups in thiolactim ethers influencing molecular conformation and the packing behavior. Journal of Molecular Structure, 2015, 1091, 88-97.	1.8	1
7073	Synergistic effect of perchlorate ions and acetonitrile medium explored for extension in copper redoximetry. Journal of Analytical Chemistry, 2015, 70, 633-638.	0.4	15
7074	Transport properties of a single-molecular diode with one backbone, and two backbones in parallel: Frontier orbital analysis and NEGF-DFT study. European Physical Journal Plus, 2015, 130, 1.	1.2	2
7075	Orthometallation of N-substituents at the NHC ligand of [Rh(Cl)(COD)(NHC)] complexes: its role in the catalytic hydrosilylation of ketones. Catalysis Science and Technology, 2015, 5, 1878-1887.	2.1	9
7076	Surface-Hopping Dynamics Simulations of Malachite Green: A Triphenylmethane Dye. Journal of Physical Chemistry A, 2015, 119, 5607-5617.	1.1	18
7077	Free electrons and ionic liquids: study of excited states by means of electron-energy loss spectroscopy and the density functional theory multireference configuration interaction method. Physical Chemistry Chemical Physics, 2015, 17, 15771-15780.	1.3	14
7078	A quantum chemical study of the factors influencing performance of DTTTD: Fullerene hetrojunction photovoltaic models. Journal of Photochemistry and Photobiology A: Chemistry, 2015, 310, 9-25.	2.0	2
7079	Novel pyrromethene dyes with N-ethyl carbazole at the meso position: a comprehensive photophysical, lasing, photostability and TD-DFT study. Physical Chemistry Chemical Physics, 2015, 17, 17221-17236.	1.3	40
7080	Interaction of rhenium(I) complex carrying long alkyl chain with Calf Thymus DNA: Cytotoxic and cell imaging studies. Inorganica Chimica Acta, 2015, 434, 51-59.	1.2	38
7081	A systematic study of chloride ion solvation in water using van der Waals inclusive hybrid density functional theory. Molecular Physics, 2015, 113, 2842-2854.	0.8	47
7082	Managing Complexity in Distributed Data Life Cycles Enhancing Scientific Discovery. , 2015, , .		10
7083	The antiradical activity of some selected flavones and flavonols. Experimental and quantum mechanical study. Journal of Molecular Modeling, 2015, 21, 307.	0.8	56
7084	Computational Examination of (4 + 3) versus (3 + 2) Cycloaddition in the Interception of Nazarov Reactions of Allenyl Vinyl Ketones by Dienes. Journal of Organic Chemistry, 2015, 80, 12535-12544.	1.7	9
7085	Noble Gas Inserted Protonated Silicon Monoxide Cations: HN _g OSi ⁺ (N _g = He, Ne, Ar, Kr,) Tj ETQq1 1 0,784314 rgBT /Overle	1.1	14
7086	NMR Investigations of Noncovalent Carbon Tetrel Bonds. Computational Assessment and Initial Experimental Observation. Journal of Physical Chemistry A, 2015, 119, 11891-11899.	1.1	88
7087	Medium-Ring Effects on the Endo/Exo Selectivity of the Organocatalytic Intramolecular Diels-Alder Reaction. Journal of Organic Chemistry, 2015, 80, 12058-12075.	1.7	11

#	ARTICLE	IF	CITATIONS
7088	Theoretical study of the structure, spectroscopic properties and anti-cancer activity of tetrahydrochromeno[4,3-b]quinolines. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550052.	1.8	3
7089	Role of the Deposition Precursor Molecules in Defining Oxidation State of Deposited Copper in Surface Reduction Reactions on H-Terminated Si(111) Surface. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27018-27027.	1.5	17
7090	Radical-induced, proton-transfer-driven fragmentations in $[b_{5} \hat{H}]E^{TM+}$ ions derived from pentaalanyl tryptophan. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10699-10707.	1.3	4
7091	H ₂ S Adsorption Characteristics on Cu ₂ O Nanostructures: A First-Principles Study. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2015, 25, 1529-1541.	1.9	3
7092	Studies on Adsorption and Corrosion Inhibitive Properties of Indoline Compounds on N80 Steel in Hydrochloric Acid. <i>Journal of Materials Engineering and Performance</i> , 2015, 24, 4975-4984.	1.2	13
7093	Photoprotection Mechanism of <i>p</i> -Methoxy Methylcinnamate: A CASPT2 Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11488-11497.	1.1	62
7094	Dibenzonaphthyridinones: Heterocycle-to-Heterocycle Synthetic Strategies and Photophysical Studies. <i>Organic Letters</i> , 2015, 17, 5732-5735.	2.4	10
7095	Nature and Catalytic Role of Extraframework Aluminum in Faujasite Zeolite: A Theoretical Perspective. <i>ACS Catalysis</i> , 2015, 5, 7024-7033.	5.5	92
7096	QM/MM study of hydrolysis of arginine catalysed by arginase. <i>Molecular Physics</i> , 0, , 1-9.	0.8	4
7097	A (pentafluoroethyl)(trifluoromethyl)carbene complex of iridium and reductive activation of its sp^3 , sp^2 , and sp carbon-fluorine bonds to give perfluoro-2-butyne, perfluoro-1,2,3-butatriene	1.6	9
7098	Novel Fluorescein-Based Fluorophores: Synthesis, Photophysics and Micro-Environmental Study. <i>Journal of Fluorescence</i> , 2015, 25, 1835-1845.	1.3	4
7099	Applications of Time-Dependent and Time-Independent Density Functional Theory to Electronic Transitions in Tetrahedral d^0 Metal Oxides. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4041-4053.	2.3	17
7100	Structure and separation quality of various N- and O-donor ligands from quantum-chemical calculations. <i>Nukleonika</i> , 2015, 60, 847-851.	0.3	10
7101	Assessing density functionals for the prediction of thermochemistry of Ti-O-Cl species. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550055.	1.8	2
7102	Static second hyperpolarizability of twisted ethylene: A comprehensive computational study. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550060.	1.8	4
7103	Mapping the HO ₃ ground state potential energy surface with DFT: Can we reproduce the MRCI+Q/CBS data?. <i>Chemical Physics Letters</i> , 2015, 620, 61-66.	1.2	4
7104	Computational Studies of a Paramagnetic Planar Dibenzotetraaza[14]annulene Ni(II) Complex. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5189-5196.	1.1	4
7105	Monoatomic-thick graphitic carbon nitride dots on graphene sheets as an efficient catalyst in the oxygen reduction reaction. <i>Nanoscale</i> , 2015, 7, 3035-3042.	2.8	85

#	ARTICLE	IF	CITATIONS
7106	Theoretical studies of Raman scattering properties of methylphosphine and methylamine adsorbed on gold clusters. <i>Vibrational Spectroscopy</i> , 2015, 76, 38-47.	1.2	5
7107	NTChem: A high-performance software package for quantum molecular simulation. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 349-359.	1.0	55
7108	Vibrational Circular Dichroism Absolute Configuration Determination of Natural Products. <i>Progress in the Chemistry of Organic Natural Products</i> , 2015, 100, 311-452.	0.8	59
7109	Catalytic Hydrodechlorination of Benzyl Chloride Promoted by Rh ⁺ -heterocyclic Carbene Catalysts. <i>ChemSusChem</i> , 2015, 8, 495-503.	3.6	15
7110	Effect of Auxiliary Chromophores on the Optical, Electrochemical, and Photovoltaic Properties of Carbazole-Based Dyes. <i>Asian Journal of Organic Chemistry</i> , 2015, 4, 69-80.	1.3	10
7111	<i>In situ</i> investigation of organic ligand displacement processes on ZnO powder surface. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 054007.	0.7	13
7112	Linear Energy Relationships in Ground State Proton Transfer and Excited State Proton-Coupled Electron Transfer. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2611-2619.	1.2	21
7113	Simulation of X-ray absorption spectra with orthogonality constrained density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14360-14374.	1.3	54
7114	Materials Meets Concepts in Molecule-Based Electronics. <i>Advanced Functional Materials</i> , 2015, 25, 1933-1954.	7.8	47
7115	Carotenoids and Light-Harvesting: From DFT/MRCI to the Tamm-Dancoff Approximation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 655-666.	2.3	44
7116	Assessment of density functionals and force field methods on anion-π interaction in heterocyclic calix complexes. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	9
7117	Design, synthesis and metal sensing studies of ether-linked bis-triazole derivatives. <i>New Journal of Chemistry</i> , 2015, 39, 3777-3784.	1.4	13
7118	Aryl-substituted symmetrical and unsymmetrical benzothiadiazoles. <i>RSC Advances</i> , 2015, 5, 18288-18294.	1.7	18
7119	Molecular modeling and experimental studies on structure and NMR parameters of 9-benzyl-3,6-diiodo-9H-carbazole. <i>Structural Chemistry</i> , 2015, 26, 997-1006.	1.0	18
7120	Theoretical analysis of [5.5.6]cyclacenes: electronic properties, strain energies and substituent effects. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7366-7372.	1.3	27
7121	Theoretical study on the stability of double-decker type metal phthalocyanines, M(Pc) ₂ and M(Pc) ₂ ⁺ (M = Ti, Sn and Sc): a critical assessment on the performance of density functionals. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6478-6483.	1.3	9
7122	A DFT study on Cu(I) coordination in Cu-ZSM-5: Effects of the functional choice and tuning of the ONIOM approach. <i>Journal of Computational Chemistry</i> , 2015, 36, 660-669.	1.5	12
7123	Theoretical study of stereoselectivity of the [1 + 2] cycloaddition reaction between (1S,3R,8S)-2,2-dichloro-3,7,7,10-tetramethyltricyclo[6,4,0,0,1.3]dodec-9-ene and dibromocarbene using density functional theory (DFT) B3LYP/6-31G*(d). <i>Journal of Molecular Modeling</i> , 2015, 21, 44.	0.8	13

#	ARTICLE	IF	CITATIONS
7124	Electronic properties of the AsCO, AsSiO and AsGeO radicals: Linear or cyclic?. <i>Polyhedron</i> , 2015, 89, 160-167.	1.0	10
7125	A Hybrid Quantum Mechanical Approach: Intimate Details of Electron Transfer between Type-I CdSe/ZnS Quantum Dots and an Anthraquinone Molecule. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7651-7658.	1.2	23
7126	Conformational properties of 1,4- and 1,5-substituted 1,2,3-triazole amino acids – building units for peptidic foldamers. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 2776-2785.	1.5	19
7127	Density Functional Theory and Hydrogen Bonds: Are We There Yet?. <i>ChemPhysChem</i> , 2015, 16, 978-985.	1.0	129
7128	Establishing the Steric Bulk of Main Group Hydrides in Reduction Reactions. <i>Israel Journal of Chemistry</i> , 2015, 55, 226-234.	1.0	8
7129	Possible use of BN-modified fullerene as a nano-biosensor to detect adenine–thymine Watson–Crick base pair in mutagenic tautomeric form: Theoretical approach. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550003.	1.8	3
7130	Role of Fluoride in Accelerating the Reactions of Dialkylstannylene Acetals. <i>Journal of Organic Chemistry</i> , 2015, 80, 2989-3002.	1.7	6
7131	Kinetic Ion Thermometers for Electron Transfer Dissociation. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2818-2826.	1.2	28
7132	Probing Peptide Cation–Radicals by Near-UV Photodissociation in the Gas Phase. Structure Elucidation of Histidine Radical Chromophores Formed by Electron Transfer Reduction. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3948-3961.	1.2	20
7133	Interpretation of the Longitudinal ¹³ C Nuclear Spin Relaxation and Chemical Shift Data for Five Bromoazaheterocycles Supported by Nonrelativistic and Relativistic DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 517-524.	1.1	2
7134	Coupled-Cluster Studies of Extensive Green Fluorescent Protein Models Using the Reduced Virtual Space Approach. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2933-2945.	1.2	30
7135	The Energy Difference between the Triply-Bridged and All-Terminal Structures of Co ₄ (CO) ₁₂ , Rh ₄ (CO) ₁₂ , and Ir ₄ (CO) ₁₂ : A Difficult Test for Conventional Density Functional Methods. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 940-949.	2.3	2
7136	Multiple Environment Single System Quantum Mechanical/Molecular Mechanical (MESS-QM/MM) Calculations. 1. Estimation of Polarization Energies. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1511-1523.	1.1	23
7137	Coupled-Perturbed SCF Approach for Calculating Static Polarizabilities and Hyperpolarizabilities with Nonorthogonal Localized Molecular Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 923-931.	2.3	2
7138	Representation of Ion–Protein Interactions Using the Drude Polarizable Force-Field. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9401-9416.	1.2	101
7139	The Coupling between Stability and Ion Pair Formation in Magnesium Electrolytes from First-Principles Quantum Mechanics and Classical Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2015, 137, 3411-3420.	6.6	259
7140	4-Pyridyl-9,9-dimethyl-spirofluorenes as Host Materials for Green and Sky-Blue Phosphorescent OLEDs. <i>Journal of Physical Chemistry C</i> , 2015, 119, 5790-5805.	1.5	59
7141	Initial Gas Phase Reactions between Al(CH ₃) ₃ /AlH ₃ and Ammonia: Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 744-751.	1.1	17

#	ARTICLE	IF	CITATIONS
7142	Ultrafast Photoinduced Electron Transfer from Peroxide Dianion. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7422-7429.	1.2	12
7143	Spin Adapted versus Broken Symmetry Approaches in the Description of Magnetic Coupling in Heterodinuclear Complexes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1006-1019.	2.3	14
7144	Activation of B–H, Si–H, and C–F Bonds with Tp–Rh(PMe ₃) ₃ Complexes: Kinetics, Mechanism, and Selectivity. <i>Journal of the American Chemical Society</i> , 2015, 137, 1258-1272.	6.6	39
7145	Computational Study on the Effect of Exocyclic Substituents on the Ionization Potential of Primaquine: Insights into the Design of Primaquine-Based Antimalarial Drugs with Less Methemoglobin Generation. <i>Chemical Research in Toxicology</i> , 2015, 28, 169-174.	1.7	6
7146	Embedded Mean-Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 568-580.	2.3	83
7147	Comparison of Real-Time and Linear-Response Time-Dependent Density Functional Theories for Molecular Chromophores Ranging from Sparse to High Densities of States. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1102-1109.	2.3	98
7148	Origins of Hydration Differences in Homochiral and Racemic Crystals of Aspartic Acid. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1396-1403.	1.1	7
7149	Theoretical Study on the Reactions of (CF ₃) ₂ CFOCH ₃ + OH/Cl and Reaction of (CF ₃) ₂ CFOCHO with Cl Atom. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1256-1266.	1.1	15
7150	Exploring the Aqueous Vertical Ionization of Organic Molecules by Molecular Simulation and Liquid Microjet Photoelectron Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2015, 119, 238-256.	1.2	32
7151	Ferrocenyl thiazoles: synthesis and properties. <i>Tetrahedron Letters</i> , 2015, 56, 1664-1666.	0.7	19
7152	Accurate reaction barrier heights of pericyclic reactions: Surprisingly large deviations for the CBS–QB3 composite method and their consequences in DFT benchmark studies. <i>Journal of Computational Chemistry</i> , 2015, 36, 622-632.	1.5	124
7153	Role of Topological Charge Stabilization in Protomeric Tautomerism. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1074-1086.	1.1	12
7154	Bicyclobutonium Ions in Biosynthesis – Interconversion of Cyclopropyl-Containing Sterols from Orchids. <i>Journal of the American Chemical Society</i> , 2015, 137, 2085-2088.	6.6	22
7155	UV-vis and EPR spectroelectrochemical investigations of triarylamine functionalized arylene bisimides. <i>RSC Advances</i> , 2015, 5, 7401-7412.	1.7	27
7156	π-Delocalization and the Vibrational Spectroscopy of Conjugated Materials: Computational Insights on Raman Frequency Dispersion in Thiophene, Furan, and Pyrrole Oligomers. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3583-3594.	1.2	36
7157	Native point defects in few-layer phosphorene. <i>Physical Review B</i> , 2015, 91, .	1.1	104
7158	Mechanism for the Nonadiabatic Photooxidation of Benzene to Phenol: Orientation-Dependent Proton-Coupled Electron Transfer. <i>ChemPhysChem</i> , 2015, 16, 933-937.	1.0	17
7159	Encapsulation of an f-block metal atom/ion to enhance the stability of C ₂₀ with the I _h symmetry. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4328-4336.	1.3	12

#	ARTICLE	IF	CITATIONS
7160	Synthesis, Structure, and Reactivity of Pentamethylcyclopentadienyl 2,4,6-Triphenylphosphinine Iron Complexes. <i>Organometallics</i> , 2015, 34, 622-635.	1.1	14
7161	Molecular magnets and surfaces: A promising marriage. A DFT insight. <i>Coordination Chemistry Reviews</i> , 2015, 289-290, 357-378.	9.5	55
7162	Assessment of Several DFT Functionals in Calculation of the Reduction Potentials for Ni ^{II} , Pd ^{II} , and Pt ^{II} Bis-ethylene-1,2-dithiolene and -Diselenolene Complexes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 911-918.	1.1	25
7163	Anandamide Hydrolysis in FAAH Reveals a Dual Strategy for Efficient Enzyme-Assisted Amide Bond Cleavage via Nitrogen Inversion. <i>Journal of Physical Chemistry B</i> , 2015, 119, 789-801.	1.2	36
7164	Study of structures, energies and vibrational frequencies of (O ₂) _n (n=2-5) clusters by GGA and meta-GGA density functional methods. <i>Computational and Theoretical Chemistry</i> , 2015, 1056, 24-36.	1.1	4
7165	Computational study of diketopyrrolopyrrole-based organic dyes for dye sensitized solar cell applications. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 57, 62-69.	1.3	16
7166	Strong Electronic Coupling Dominates the Absorption and Fluorescence Spectra of Covalently Bound BisBODIPYs. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1323-1331.	1.1	25
7167	Solvent effects in time-dependent self-consistent field methods. I. Optical response calculations. <i>Journal of Chemical Physics</i> , 2015, 142, 044103.	1.2	28
7168	Density functional theory (DFT) as a powerful tool for designing new organic corrosion inhibitors. Part 1: An overview. <i>Corrosion Science</i> , 2015, 99, 1-30.	3.0	807
7169	Comparison of direct dynamics simulations with different electronic structure methods. F ⁺ + CH ₃ I with MP2 and DFT/B97-1. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2589-2597.	1.3	47
7170	Brønsted and Lewis acid sites of Sn-beta zeolite, in combination with the borate salt, catalyze the epimerization of glucose: A density functional theory study. <i>Journal of Catalysis</i> , 2015, 323, 158-164.	3.1	31
7171	Efficient and Selective Palladium-Catalysed C ₃ Urea Couplings to 3,5-Dichloro(1 <i>H</i>)pyrazinones. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 978-986.	1.2	10
7172	Polymer nanocomposite fiber model interphases: Influence of processing and interface chemistry on mechanical performance. <i>Chemical Engineering Journal</i> , 2015, 269, 121-134.	6.6	55
7173	Encapsulation of Xenon by a Self-Assembled Fe ₄ L ₆ Metallosupramolecular Cage. <i>Journal of the American Chemical Society</i> , 2015, 137, 2464-2467.	6.6	89
7174	Systematic Strategy for Designing Imidazolium Containing Precursors To Produce <i>i</i> -N-Heterocyclic Carbenes: A DFT Study. <i>Journal of Organic Chemistry</i> , 2015, 80, 1878-1886.	1.7	5
7175	Natural Abundance ¹⁵ N-NMR by Dynamic Nuclear Polarization: Fast Analysis of Binding Sites of a Novel Amine-Carboxyl-Linked Immobilized Dirhodium Catalyst. <i>Chemistry - A European Journal</i> , 2015, 21, 3798-3805.	1.7	59
7176	NLO Properties of Unidirectional Lengthening [Pt ₃ (CO) ₃ (½-CO) ₃] _n Clusters: A TDDFT Study. <i>Journal of Cluster Science</i> , 2015, 26, 1511-1526.	1.7	0
7177	New Tetracobalt Cluster Compounds for Electrocatalytic Proton Reduction: Syntheses, Structures, and Reactivity. <i>Chemistry - A European Journal</i> , 2015, 21, 4027-4038.	1.7	2

#	ARTICLE	IF	CITATIONS
7178	High-Quality Thermochemistry Data on Polycyclic Aromatic Hydrocarbons via Quantum Chemistry. <i>Polycyclic Aromatic Compounds</i> , 2015, 35, 16-31.	1.4	2
7179	Two novel unsymmetrical ferrocene based azines and their complexing abilities towards Cu(II): Spectroscopy, crystal structure, electrochemistry and DFT calculations. <i>Polyhedron</i> , 2015, 88, 182-189.	1.0	18
7180	Conformational study of some 4- R^2 -substituted 2-(phenylselanyl)-2-(ethylsulfonyl)-acetophenones. <i>Journal of Molecular Structure</i> , 2015, 1084, 190-199.	1.8	3
7181	Computational Photochemistry of the Azobenzene Scaffold of Sudan I and Orange II Dyes: Excited-State Proton Transfer and Deactivation via Conical Intersections. <i>ChemPhysChem</i> , 2015, 16, 805-811.	1.0	29
7182	Mechanistic Aspects of the Gas-Phase Reactions of Halobenzenes with Bare Lanthanide Cations: A Combined Experimental/Theoretical Investigation. <i>Chemistry - A European Journal</i> , 2015, 21, 2123-2131.	1.7	13
7183	Applications of Time-Dependent and Time-Independent Density Functional Theory to Rydberg Transitions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5107-5116.	1.1	20
7184	Efficient Implementation of the Pair Atomic Resolution of the Identity Approximation for Exact Exchange for Hybrid and Range-Separated Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 518-527.	2.3	46
7185	DFT Study on the Impact of the Methylaluminoxane Cocatalyst in Ethylene Oligomerization Using a Titanium-Based Catalyst. <i>Organometallics</i> , 2015, 34, 426-431.	1.1	15
7186	Origins of the Regioselectivity in the Lutetium Triflate Catalyzed Ketalization of Acetone with Glycerol: A DFT Study. <i>ACS Catalysis</i> , 2015, 5, 1013-1019.	5.5	24
7187	Unravelling the Quenching Mechanisms of a Luminescent Ru(II) Probe for Cu(II). <i>Chemistry - an Asian Journal</i> , 2015, 10, 622-629.	1.7	10
7188	Conformational study of some 4- R^2 -substituted 2-(phenylselanyl)-2-(ethylsulfonyl)-acetophenones. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 495-504.	2.0	4
7189	Fluorene-Based Sensitizers with a Phenothiazine Donor: Effect of Mode of Donor Tethering on the Performance of Dye-Sensitized Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 2249-2262.	4.0	84
7190	The number density effect of N-substituted dyes on the TiO ₂ surface in dye sensitized solar cells: a theoretical study. <i>RSC Advances</i> , 2015, 5, 11549-11557.	1.7	12
7191	High-Level Ab Initio Computations of the Absorption Spectra of Organic Iridium Complexes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1023-1036.	1.1	34
7192	The effect of TiO ₂ surface on the electron injection efficiency in PbS quantum dot solar cells: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6076-6086.	1.3	20
7193	Iridium Half-Sandwich Complexes with Di- and Tridentate Bis(pyridylimino)isoindolato Ligands: Stoichiometric and Catalytic Reactivity. <i>Organometallics</i> , 2015, 34, 2326-2342.	1.1	22
7194	Heteroleptic Ru(II)-terpyridine complex and its metal-containing conducting polymer: Synthesis and characterization. <i>Synthetic Metals</i> , 2015, 200, 109-116.	2.1	5
7195	QM/QM Approach to Model Energy Disorder in Amorphous Organic Semiconductors. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 560-567.	2.3	40

#	ARTICLE	IF	CITATIONS
7196	Insights into the preferential order of strand exchange in the Cre/loxP recombinase system: impact of the DNA spacer flanking sequence and flexibility. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 271-282.	1.3	7
7197	Intrinsic interfacial phenomena in manganite heterostructures. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 123001.	0.7	25
7198	Intriguing radical-radical interactions among double-electron oxidized adenine-thymine base pairs. <i>Chemical Physics Letters</i> , 2015, 619, 223-229.	1.2	6
7199	Molecular modeling reveals binding interface of β -tubulin with GCP4 and interactions with noscapinoids. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 827-843.	1.5	10
7200	DFT Study of the Molybdenum-Catalyzed Deoxydehydration of Vicinal Diols. <i>Chemistry - A European Journal</i> , 2015, 21, 3435-3442.	1.7	38
7201	Electron Transfer Reduction of the Diazirine Ring in Gas-Phase Peptide Ions. On the Peculiar Loss of $[\text{NH}_4\text{O}]$ from Photoleucine. <i>Journal of the American Society for Mass Spectrometry</i> , 2015, 26, 415-431.	1.2	9
7202	Computational evidence for structural consequences of kiteplatin damage on DNA. <i>Journal of Biological Inorganic Chemistry</i> , 2015, 20, 35-48.	1.1	12
7203	Total energy equation leading to exchange-correlation functional. <i>Science China: Physics, Mechanics and Astronomy</i> , 2015, 58, 1-6.	2.0	0
7204	Theoretical and kinetic study of reaction $\text{C}_2\text{H} + \text{C}_3\text{H}_6$ on the C_5H_7 potential energy surface. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	12
7205	Photophysical Properties of β -Substituted Free-Base Corroles. <i>Inorganic Chemistry</i> , 2015, 54, 2713-2725.	1.9	47
7206	A molecular level mechanism for uranium (VI) toxicity through Ca^{2+} displacement in pyrroloquinoline quinone-dependent bacterial dehydrogenase. <i>Journal of Inorganic Biochemistry</i> , 2015, 149, 59-67.	1.5	7
7207	Theoretical investigation on the electronic structure and phosphorescent properties of a series of blue iridium ($\text{Ir}(\text{acac})_3$) complexes with the 2-phenylpyridine ligands. <i>Journal of Organometallic Chemistry</i> , 2015, 785, 44-51.	0.8	7
7208	Remote Substituent Effects on the Stereoselectivity and Organocatalytic Activity of Densely Substituted Unnatural Proline Esters in Aldol Reactions. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 2503-2516.	1.2	23
7209	Sources of n -type conductivity in GaInO_3 . <i>Journal Physics D: Applied Physics</i> , 2015, 48, 015101.	1.3	13
7210	Infrared spectroscopic and theoretical study of the reactions of cerium atoms with methanol in solid argon. <i>Journal of Molecular Spectroscopy</i> , 2015, 310, 50-56.	0.4	10
7211	Charge transfer or biradicaloid character: assessing TD-DFT and SAC-CI for squarylium dye derivatives. <i>RSC Advances</i> , 2015, 5, 18813-18821.	1.7	12
7212	Molecular engineering of quinoxaline dyes toward more efficient sensitizers for dye-sensitized solar cells. <i>RSC Advances</i> , 2015, 5, 25079-25088.	1.7	26
7213	Quantifying Reactivity for Electrophilic Aromatic Substitution Reactions with Hirshfeld Charge. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3107-3111.	1.1	74

#	ARTICLE	IF	CITATIONS
7214	Electronic structure and optical properties of $\text{Fe}_{1-x}\text{V}_x\text{O}_3$ solid-solution thin films. <i>Applied Physics Letters</i> , 2015, 106, .	1.5	13
7215	Calculated Nuclear Magnetic Resonance Spectra of Polytwistane and Related Hydrocarbon Nanorods. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1020-1026.	2.3	7
7216	Phenanthrene Condensed Thiadiazoloquinoxaline Donor-Acceptor Polymer for Phototransistor Applications. <i>Chemistry of Materials</i> , 2015, 27, 2218-2223.	3.2	67
7217	Deviations from piecewise linearity in the solid-state limit with approximate density functionals. <i>Journal of Chemical Physics</i> , 2015, 142, 034107.	1.2	42
7218	Theoretical investigations of the perylene electronic structure: Monomer, dimers, and excimers. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 442-452.	1.0	57
7219	A new multicomponent salt of imidazole and tetrabromoterephthalic acid: Structural, optical, thermal, electrical transport properties and antibacterial activity along with Hirshfeld surface analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 144, 43-52.	2.0	13
7220	Quantum Chemical Investigation of <i>meta</i> -Xylylene Based One-Dimensional Polymer Chain. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2176-2185.	1.1	8
7221	Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. <i>Journal of Chemical Physics</i> , 2015, 142, 034111.	1.2	17
7222	All-electron formalism for total energy strain derivatives and stress tensor components for numeric atom-centered orbitals. <i>Computer Physics Communications</i> , 2015, 190, 33-50.	3.0	92
7223	Computational Exploration of Conformations of Glycine-Arginine and a Deduced Model on Global Minimum Configurations of Dipeptides in Gas Phase. <i>Chinese Journal of Chemical Physics</i> , 2015, 28, 161-167.	0.6	6
7224	Unusual photophysical properties of conjugated, alternating indigo-fluorene copolymers. <i>Journal of Materials Chemistry A</i> , 2015, 3, 6373-6382.	5.2	24
7225	Electronic and optical properties of reduced graphene oxide. <i>Journal of Materials Chemistry C</i> , 2015, 3, 7632-7641.	2.7	78
7226	Water splitting with polyoxometalate-treated photoanodes: enhancing performance through sensitizer design. <i>Chemical Science</i> , 2015, 6, 5531-5543.	3.7	67
7227	Mechanistic Insights into the Cu(I)- and Cu(II)-Catalyzed Cyclization of <i>o</i> -Alkynylbenzaldehydes: The Solvent DMF and Oxidation State of Copper Affect the Reaction Mechanism. <i>Journal of Organic Chemistry</i> , 2015, 80, 6553-6563.	1.7	21
7228	Reaction barrier heights for cycloreversion of heterocyclic rings: An Achilles' heel for DFT and standard ab initio procedures. <i>Chemical Physics</i> , 2015, 458, 1-8.	0.9	68
7229	Experimental and theoretical studies of hydrolysis of nerve agent sarin by binuclear zinc biomimetic catalysts. <i>Chemical Physics</i> , 2015, 457, 70-77.	0.9	7
7230	Synthesis, chemical characterization, computational studies and biological activity of new DNA methyltransferases (DNMTs) specific inhibitor. Epigenetic regulation as a new and potential approach to cancer therapy. <i>Journal of Inorganic Biochemistry</i> , 2015, 150, 18-27.	1.5	14
7231	Photophysical and theoretical studies on newly synthesized N,N-diphenylamine based azo dye. <i>Journal of Molecular Structure</i> , 2015, 1099, 543-550.	1.8	15

#	ARTICLE	IF	CITATIONS
7232	Colorimetric and fluorimetric detection of fluoride and cyanide ions using tri and tetra coordinated boron containing chromophores. Dalton Transactions, 2015, 44, 16052-16060.	1.6	44
7233	Intermolecular heterocyclization of alkynones with 2-mercaptoacetaldehyde under metal-free conditions: synthesis of 2,3-disubstituted thiophenes. Tetrahedron Letters, 2015, 56, 5386-5389.	0.7	13
7234	Quantum-Chemical Studies on Excitation Energy Transfer Processes in BODIPY-Based Donor-Acceptor Systems. Journal of Chemical Theory and Computation, 2015, 11, 4316-4327.	2.3	29
7235	Resolution and Determination of the Absolute Configuration of a Twisted Bis-Lactam Analogue of Tröger's Base: A Comparative Spectroscopic and Computational Study. Journal of Organic Chemistry, 2015, 80, 8142-8149.	1.7	11
7236	Adsorption of Dilute Alcohols onto Cyclodextrin-Polysulfone Membrane: Experimental and Theoretical Analysis. Journal of Chemical & Engineering Data, 2015, 60, 2549-2558.	1.0	4
7237	DFT investigation on interaction of chlorine with In ₂ O ₃ nanostructures. Canadian Journal of Chemistry, 2015, 93, 1249-1260.	0.6	2
7238	Catalytic sugar-assisted transfer hydrogenation with Ru(II), Rh(III) and Ir(III) halfsandwich complexes. Journal of Molecular Catalysis A, 2015, 408, 107-122.	4.8	3
7239	Screened Hybrid Exact Exchange Correction Scheme for Adsorption Energies on Perovskite Oxides. Journal of Physical Chemistry C, 2015, 119, 17662-17666.	1.5	7
7240	Silicon isotope fractionation during the precipitation of quartz and the adsorption of H ₄ SiO ₄ (aq) on Fe(III)-oxyhydroxide surfaces. Diqiu Huaxue, 2015, 34, 459-468.	0.5	23
7241	Iridium complexes as catalysts in the hydrogen transfer of isopropanol to acetophenone: Ligand effects and DFT studies. Inorganica Chimica Acta, 2015, 436, 146-151.	1.2	14
7242	Theoretical and experimental study on intramolecular charge-transfer in symmetric bi-1,3,4-oxadiazole derivatives. Journal of Photochemistry and Photobiology A: Chemistry, 2015, 312, 20-27.	2.0	29
7243	Metallophilic Contacts in 2-C ₆ F ₄ PPH ₂ Bridged Heterobinuclear Complexes: A Crystallographic and Computational Study. Inorganic Chemistry, 2015, 54, 6947-6957.	1.9	13
7244	Conjugate Addition/[3,3] Sigmatropic Shift Processes for Formation of Medium-Ring Cyclic Amines - Do They Circumvent the Woodward-Hoffmann Rules?. Journal of Organic Chemistry, 2015, 80, 11699-11705.	1.7	8
7245	Study on Synthesis and Fluorescence of Novel Benzofused Phenazine π -Conjugated Skeleton with Coumarin and Isophoron Cores. Journal of Fluorescence, 2015, 25, 1095-1102.	1.3	4
7246	Dinuclear iridium and rhodium complexes with bridging arylimidazolide-N ³ ,C ² ligands: synthetic, structural, reactivity, electrochemical and spectroscopic studies. Dalton Transactions, 2015, 44, 17030-17044.	1.6	15
7247	Fluorescence Enhancement/Quenching Based on Metal Orbital Control: Computational Studies of a 6-Thienylumazine-Based Mercury Sensor. Journal of Physical Chemistry A, 2015, 119, 8106-8116.	1.1	49
7248	Electronic and Chemical State of Aluminum from the Single- (K) and Double-Electron Excitation (KL _{II&III} , KL _I) X-ray Absorption Near-Edge Spectra of \pm -Alumina, Sodium Aluminate, Aqueous Al ³⁺ ·(H ₂ O) ₆ , and Aqueous Al(OH) ₄ ⁻ . Journal of Physical Chemistry B, 2015, 119, 8380-8388.	1.2	20
7249	Understanding reactivity and regioselectivity in Diels-Alder reactions of a sugar-derived dienophile bearing two competing EWGs. An experimental and computational study. Carbohydrate Research, 2015, 415, 54-59.	1.1	2

#	ARTICLE	IF	CITATIONS
7250	Assessment of Empirical Models versus High-Accuracy Ab Initio Methods for Nucleobase Stacking: Evaluating the Importance of Charge Penetration. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4197-4204.	2.3	51
7251	Selectivity and mechanism of thermal decomposition of β^2 -diketones on ZnO powder. <i>Journal of Catalysis</i> , 2015, 330, 145-153.	3.1	13
7252	Virtual Screening for Transition State Analogue Inhibitors of IRAP Based on Quantum Mechanically Derived Reaction Coordinates. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1984-1993.	2.5	9
7253	Benchmarking Continuum Solvent Models for Keto \rightleftharpoons Enol Tautomerizations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8724-8733.	1.1	25
7254	Structure and electronic properties of MoVO type mixed-metal oxides \rightleftharpoons a combined view by experiment and theory. <i>Dalton Transactions</i> , 2015, 44, 13778-13795.	1.6	21
7255	Computational investigation on the intramolecular resonance-inhibited hydrogen bonding: a new type of interaction versus the RAHB model. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	12
7256	Kinetics of the Addition of Olefins to Si-Centered Radicals: The Critical Role of Dispersion Interactions Revealed by Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5883-5888.	1.1	5
7257	Computational Study of Chemical Reactivity Using Information-Theoretic Quantities from Density Functional Reactivity Theory for Electrophilic Aromatic Substitution Reactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8216-8224.	1.1	43
7258	Positional Isomers of Tetramethoxyppyrene-based Mono- and Biradicals. <i>Journal of Physical Chemistry B</i> , 2015, 119, 13649-13655.	1.2	8
7259	Characterization of the Dielectric Constant in the <i>Trichoderma reesei</i> Cel7B Active Site. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1369-1376.	2.5	5
7260	Stacked and H-Bonded Cytosine Dimers. Analysis of the Intermolecular Interaction Energies by Parallel Quantum Chemistry and Polarizable Molecular Mechanics. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9477-9495.	1.2	19
7262	Redox Photocatalysis with Water-Soluble Core \rightleftharpoons Shell CdSe-ZnS Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2015, 119, 17857-17866.	1.5	22
7263	Performance of the M06 family of functionals in predicting the charge transfer transition energies of molecular complexes of TCNE with a series of methylated indoles. <i>Computational and Theoretical Chemistry</i> , 2015, 1068, 123-127.	1.1	4
7264	High-resolution X-ray absorption spectroscopy of iron carbonyl complexes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13937-13948.	1.3	36
7265	Active space and basis set effects in CASPT_2 models of the 1,3-butadiene \rightleftharpoons ethene cycloaddition and the 1,3-butadiene dimerization. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 989-1001.	1.0	4
7266	Gas \rightleftharpoons phase ammonia activation by Th, Th ⁺ , and Th ²⁺ : Reaction mechanisms, bonding analysis, and rate constant calculations. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 6-18.	1.0	15
7267	First \rightleftharpoons principles approaches for strongly correlated materials: A theoretical chemistry perspective. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 722-730.	1.0	31
7268	On the Performance of Optimally Tuned Range-Separated Hybrid Functionals for X-ray Absorption Modeling. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3234-3244.	2.3	20

#	ARTICLE	IF	CITATIONS
7269	Density Functional Theory Study of BF ₃ -Mediated Additions of Enols and [(Trimethylsilyl)oxy]alkenes to an Oxyallyl Cation: Homologous Mukaiyama Reactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6714-6722.	1.1	6
7270	Energetics, thermal isomerisation and photochemistry of the linkage-isomer system [Ni(Et ₄ dien)(² -O,ON)(¹ -NO ₂)]. <i>CrystEngComm</i> , 2015, 17, 383-394.	1.3	16
7271	Multiple active zones in hybrid QM/MM molecular dynamics simulations for large biomolecular systems. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9959-9972.	1.3	11
7272	Nickel(II) radical complexes of thiosemicarbazone ligands appended by salicylidene, aminophenol and aminothiophenol moieties. <i>Dalton Transactions</i> , 2015, 44, 12743-12756.	1.6	24
7273	A Quantum Chemical and Statistical Study of Cytotoxic Activity of Compounds Isolated from <i>Curcuma zedoaria</i> . <i>International Journal of Molecular Sciences</i> , 2015, 16, 9450-9468.	1.8	11
7274	Variational Optimization of the Second-Order Density Matrix Corresponding to a Seniority-Zero Configuration Interaction Wave Function. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4064-4076.	2.3	46
7275	A Chemically Meaningful Measure of Electron Localization. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3617-3628.	2.3	14
7276	Mechanism and stereoselectivity of the Rh(II)-catalyzed cyclopropanation of diazooxindole: a density functional theory study. <i>RSC Advances</i> , 2015, 5, 57781-57791.	1.7	31
7277	Spacer controlled photo-induced intramolecular electron transfer in a series of phenothiazine-boron dipyrromethene donor-acceptor dyads. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2015, 312, 8-19.	2.0	34
7278	Handling Magnetic Coupling in Trinuclear Cu(II) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3650-3660.	2.3	13
7279	Hybrid Functionals with Variationally Fitted Exact Exchange. <i>Advances in Quantum Chemistry</i> , 2015, 71, 41-67.	0.4	11
7280	Vibrational Properties of the Phosphate Group Investigated by Molecular Dynamics and Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10682-10692.	1.2	23
7281	The Importance of the MM Environment and the Selection of the QM Method in QM/MM Calculations. <i>Advances in Protein Chemistry and Structural Biology</i> , 2015, 100, 153-185.	1.0	2
7282	Nitric Oxide Catalysis of Diazene E/Z Isomerization. <i>Inorganic Chemistry</i> , 2015, 54, 7145-7151.	1.9	6
7283	Understanding the conformational behaviour of Ac-Ala-NHMe in different media. A joint NMR and DFT study. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 9206-9213.	1.5	11
7284	Performance of Frozen Density Embedding for Modeling Hole Transfer Reactions. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7541-7557.	1.2	46
7285	A new insight on the gas phase retro-Diels-Alder reaction of bicyclic compounds: density functional theory calculations. <i>Molecular Physics</i> , 2015, 113, 3182-3195.	0.8	2
7286	Group Additive Kinetics for Hydrogen Transfer Between Oxygenates. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6961-6980.	1.1	16

#	ARTICLE	IF	CITATIONS
7287	Joint Experimental, in Silico, and NMR Studies toward the Rational Design of Iminium-Based Organocatalyst Derived from Renewable Sources. <i>Journal of Organic Chemistry</i> , 2015, 80, 7626-7634.	1.7	28
7288	Monitoring the intramolecular charge transfer process in the Z907 solar cell sensitizer: a transient Vis and IR spectroscopy and ab initio investigation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 21594-21604.	1.3	10
7289	Impact of structural differences in carcinopreventive agents indole-3-carbinol and 3,3'-diindolylmethane on biological activity. An X-ray, ^1H NMR, ^{13}C CP/MAS NMR, and periodic hybrid DFT study. <i>European Journal of Pharmaceutical Sciences</i> , 2015, 77, 141-153.	1.9	4
7290	The electronic structure engineering of organic dye sensitizers for solar cells: The case of JK derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 855-866.	2.0	6
7291	Revisiting the beryllium bonding interactions from energetic and wavefunction perspectives. <i>Chemical Physics Letters</i> , 2015, 633, 265-272.	1.2	17
7292	Calibration of Energy-Specific TDDFT for Modeling K-edge XAS Spectra of Light Elements. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2994-2999.	2.3	78
7293	Formation of 5-(Hydroxymethyl)furfural by Stepwise Dehydration over TiO_2 with Water-Tolerant Lewis Acid Sites. <i>Journal of Physical Chemistry C</i> , 2015, 119, 17117-17125.	1.5	82
7294	Interplay of Experiment and Theory in Elucidating Mechanisms of Oxidation Reactions by a Nonheme $\text{Ru}^{\text{IV}}\text{O}$ Complex. <i>Journal of the American Chemical Society</i> , 2015, 137, 8623-8632.	6.6	85
7295	Complexation of uranium(VI) with glutarimidooxime: thermodynamic and computational studies. <i>Dalton Transactions</i> , 2015, 44, 13835-13844.	1.6	54
7296	Modeling $\text{Cu}^{2+}\text{-Al}^2$ complexes from computational approaches. <i>AIP Advances</i> , 2015, 5, 092402.	0.6	17
7297	The importance of current contributions to shielding constants in density-functional theory. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 18834-18842.	1.3	35
7298	Gas Phase Studies of N-Heterocyclic Carbene-Catalyzed Condensation Reactions. <i>Journal of Organic Chemistry</i> , 2015, 80, 6831-6838.	1.7	11
7299	Screening novel candidates and exploring design strategies for organic dye sensitizers with rigid π -linker: A theoretical study. <i>Materials Chemistry and Physics</i> , 2015, 162, 700-710.	2.0	12
7300	Localized Excitation of Ti^{3+} Ions in the Photoabsorption and Photocatalytic Activity of Reduced Rutile TiO_2 . <i>Journal of the American Chemical Society</i> , 2015, 137, 9146-9152.	6.6	168
7301	Water-catalysis in the gas phase reaction of dithioformic acid with hydroxyl radical: global reaction route mapping of oxidative pathways for hydrogen abstraction. <i>RSC Advances</i> , 2015, 5, 50989-50998.	1.7	6
7302	Quantum chemistry based calibration of the alkali metal cation series (Li^+ ; Cs^+) for large-scale polarizable molecular mechanics/dynamics simulations. <i>Journal of Computational Chemistry</i> , 2015, 36, 285-302.	1.5	12
7303	Substituent effects in the Diels-Alder reactions of butadienes, cyclopentadienes, furans and pyrroles with maleic anhydride. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 370-376.	0.9	14
7304	Molecular simulation of multi-component adsorption processes related to carbon capture in a high surface area, disordered activated carbon. <i>Carbon</i> , 2015, 94, 27-40.	5.4	38

#	ARTICLE	IF	CITATIONS
7305	Linear optical properties of defective KDP with oxygen vacancy: First-principles calculations. Chinese Physics B, 2015, 24, 077802.	0.7	12
7306	Inverse Thio Effects in the Hepatitis Delta Virus Ribozyme Reveal that the Reaction Pathway Is Controlled by Metal Ion Charge Density. Biochemistry, 2015, 54, 2160-2175.	1.2	50
7307	Validation of Methods for Computational Catalyst Design: Geometries, Structures, and Energies of Neutral and Charged Silver Clusters. Journal of Physical Chemistry C, 2015, 119, 9617-9626.	1.5	31
7308	Metalation of Glycylglycine: An Experimental Study Performed in Tandem with Theoretical Calculations. Journal of Chemical & Engineering Data, 2015, 60, 659-673.	1.0	4
7309	Impact of Aqueous Medium on Zeolite Framework Integrity. Chemistry of Materials, 2015, 27, 3533-3545.	3.2	50
7310	Efficient Self-Consistent Implementation of Local Hybrid Functionals. Journal of Chemical Theory and Computation, 2015, 11, 1540-1548.	2.3	69
7311	Theoretical Investigation on the Reaction between OH Radical and 4,4-Dimethyl-1-pentene in the Presence of O ₂ . Journal of Physical Chemistry A, 2015, 119, 4065-4072.	1.1	9
7312	Rate coefficients for the reaction of OH radicals with cis-3-hexene: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 8714-8722.	1.3	6
7313	Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{G} \langle \text{mml:mi} \rangle \langle \text{mml:mi} \rangle \text{W} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{structure calculations and experiments. Physical Review B, 2015, 91, .$	1.1	140
7314	Serine effects on collision-induced dissociation and photodissociation of peptide cation radicals of the + $\hat{\alpha}$ -type. International Journal of Mass Spectrometry, 2015, 378, 20-30.	0.7	17
7315	Theoretical investigation of the hydrogen shift reactions in peroxy radicals derived from the atmospheric decomposition of 3-methyl-3-buten-1-ol (MBO331). Chemical Physics Letters, 2015, 619, 236-240.	1.2	19
7316	Condensed Derivatives of Thiadiazoloquinoxaline as Strong Acceptors. Crystal Growth and Design, 2015, 15, 1934-1938.	1.4	23
7317	Biochemical characterization and molecular dynamic simulation of $\hat{1}^2$ -sitosterol as a tubulin-binding anticancer agent. European Journal of Pharmacology, 2015, 760, 154-162.	1.7	24
7318	Effects of cluster size on calculation of activation energies of silicon surface reactions with H ₂ and HCl. Journal of Crystal Growth, 2015, 418, 115-119.	0.7	12
7319	Microhydration effects on geometric properties and electronic absorption spectra of ortho-aminobenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 147, 328-333.	2.0	3
7320	The 6,6- \hat{D} icyanopentafulvene Core: A Template for the Design of Electron-Acceptor Compounds. Chemistry - A European Journal, 2015, 21, 8168-8176.	1.7	13
7321	Assessing accuracy of exchange-correlation functionals for singlet-triplet excitations. Computational and Theoretical Chemistry, 2015, 1060, 52-57.	1.1	2
7322	RPF151, a novel capsaicin-like analogue: in vitro studies and in vivo preclinical antitumor evaluation in a breast cancer model. Tumor Biology, 2015, 36, 7251-7267.	0.8	18

#	ARTICLE	IF	CITATIONS
7323	Modelling proton tunnelling in the adenine-thymine base pair. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13034-13044.	1.3	54
7324	Acid-base effects, light emission, DNA-binding and photocleavage studies of oligo-homonuclear ruthenium(II) complexes and their computational study. <i>Inorganica Chimica Acta</i> , 2015, 432, 158-168.	1.2	6
7325	Dinuclear and polymeric ($\frac{1}{4}$ -formate)nickel(II) complexes: Synthesis, structure, spectral and magnetic properties. <i>Polyhedron</i> , 2015, 95, 45-53.	1.0	8
7326	Frozen-Density Embedding Strategy for Multilevel Simulations of Electronic Structure. <i>Chemical Reviews</i> , 2015, 115, 5891-5928.	23.0	258
7327	Theoretical studies on the degradation of hydrocarbon copolymer ionomers used in fuel cells. <i>Journal of Membrane Science</i> , 2015, 487, 229-239.	4.1	32
7328	Asymmetric and symmetric triazenido cyclopalladated complexes: Synthesis, structural analysis and DFT calculations. <i>Journal of Molecular Structure</i> , 2015, 1083, 311-318.	1.8	4
7329	DFT-ONIOM study of the dopamine- β -CD complex: NBO and AIM analysis. <i>Canadian Journal of Chemistry</i> , 2015, 93, 1115-1121.	0.6	11
7330	DFT study of molecular structures and ^{13}C NMR parameters of two fluorinated biphenyls and their δ -6-tricarbonylchromium complexes. <i>Journal of Molecular Structure</i> , 2015, 1091, 222-227.	1.8	5
7331	Diradical character and second hyperpolarizability of multidecker inverse sandwich complexes of Mg and Ca. <i>Chemical Physics Letters</i> , 2015, 628, 1-8.	1.2	12
7332	Quantum-Chemical Characterization of the Properties and Reactivities of Metal-Organic Frameworks. <i>Chemical Reviews</i> , 2015, 115, 6051-6111.	23.0	241
7333	Phenazine Fused Benzo Coumarins with Negative Solvatochromism and Positive Solvatochromic Emission - Synthesis, Photo Physical Properties, DFT and TDDFT Studies. <i>Journal of Fluorescence</i> , 2015, 25, 675-684.	1.3	12
7334	The Stabilizing Role of the Intramolecular C-H \cdots O Hydrogen Bond in Cyclic Amides Derived From β -Methylbenzylamine. <i>Journal of Organic Chemistry</i> , 2015, 80, 4481-4490.	1.7	27
7335	Triple bond-modified anthracene sensitizers for dye-sensitized solar cells: a computational study. <i>RSC Advances</i> , 2015, 5, 38130-38140.	1.7	33
7336	Density functional investigation of the thermophysical and thermochemical properties of talc [$\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$]. <i>Physics and Chemistry of Minerals</i> , 2015, 42, 151-162.	0.3	31
7337	Electronic structure of modeled vs. real carbon-chain containing organometallic dinuclear complexes: similarities and differences. <i>Journal of Molecular Modeling</i> , 2015, 21, 71.	0.8	8
7338	DFT Studies of the Photophysical Properties of Fluorescent and Semiconductor Polycyclic Benzimidazole Derivatives. <i>Journal of Fluorescence</i> , 2015, 25, 685-694.	1.3	13
7339	In Silico Predictions of Human Skin Permeability using Nonlinear Quantitative Structure-Property Relationship Models. <i>Pharmaceutical Research</i> , 2015, 32, 2360-2371.	1.7	40
7340	Conductivity of phosphoric acid: an in situ comparative study of proton in phosphoric acid fuel cell. <i>Ionics</i> , 2015, 21, 2583-2590.	1.2	10

#	ARTICLE	IF	CITATIONS
7341	Functionalization of N ₂ to NH ₃ via direct N–N bond cleavage using M(III)(NMe ₂) ₃ (M=W/Mo): A theoretical study. <i>Journal of Chemical Sciences</i> , 2015, 127, 83-94.	0.7	4
7342	Carbazole-based sensitizers for potential application to dye sensitized solar cells. <i>Journal of Chemical Sciences</i> , 2015, 127, 383-394.	0.7	17
7343	AlCl ₃ -Catalyzed Ring Expansion Cascades of Bicyclic Cyclobutenamides Involving Highly Strained <i>Cis</i> , <i>Trans</i> -Cycloheptadienone Intermediates. <i>Journal of the American Chemical Society</i> , 2015, 137, 5596-5601.	6.6	31
7344	Spectroscopic and Computational Studies of Cobalamin Species with Variable Lower Axial Ligation: Implications for the Mechanism of Co–C Bond Activation by Class I Cobalamin-Dependent Isomerases. <i>Inorganic Chemistry</i> , 2015, 54, 3736-3747.	1.9	21
7345	Spatial structure and electron energy spectra of ScGe _n ⁺ (n = 6–16) clusters. <i>Russian Journal of Physical Chemistry B</i> , 2015, 9, 9-18.	0.2	12
7346	Electronic Circular Dichroism of Highly Conjugated π -Systems: Breakdown of the Tamm–Dancoff/Configuration Interaction Singles Approximation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3653-3662.	1.1	23
7347	Delocalization of Charge and Electron Density in the Humulyl Cation—Implications for Terpene Biosynthesis. <i>Journal of Organic Chemistry</i> , 2015, 80, 4046-4053.	1.7	14
7348	Search for the global minimum structures of AlB ₃ H ₂ ⁺ (n = 6) clusters. <i>Journal of Computational Chemistry</i> , 2015, 36, 385-391.		
7349	Comparison between hybrid functionals free of adjustable parameters and symmetry-adapted cluster–configuration interaction for electronically excited states of organic compounds: TD-PBEO-1/3 is better than expected. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	6
7350	N-2-Aryl-1,2,3-Triazoles: A Novel Class of Blue Emitting Fluorophores—Synthesis, Photophysical Properties Study and DFT Computations. <i>Journal of Fluorescence</i> , 2015, 25, 985-996.	1.3	16
7351	Ultrafast coherent oscillations reveal a reactive mode in the ring-opening reaction of fulgides. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14045-14053.	1.3	36
7352	Structure and Chemistry of SeF _x (CN) _{4-x} Compounds. <i>Inorganic Chemistry</i> , 2015, 54, 5220-5231.	1.9	12
7353	Include Dispersion in Quantum Chemical Modeling of Enzymatic Reactions: The Case of Isoaspartyl Dipeptidase. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2525-2535.	2.3	23
7354	Investigation of Fragmentation of Tryptophan Nitrogen Radical Cation. <i>Journal of the American Society for Mass Spectrometry</i> , 2015, 26, 1388-1393.	1.2	8
7355	Experimental and Computational Mechanistic Investigation of Chlorocarbene Additions to Bridgehead Carbene–Anti-Bredt Systems: Noradamantylcarbene–Adamantene and Adamantylcarbene–Homoadamantene. <i>Journal of Organic Chemistry</i> , 2015, 80, 5049-5065.	1.7	10
7356	Technical advances in molecular simulation since the 1980s. <i>Archives of Biochemistry and Biophysics</i> , 2015, 582, 3-9.	1.4	12
7357	Synthesis and application of new acetohydrazide derivatives as a corrosion inhibition of mild steel in acidic medium: Insight from electrochemical and theoretical studies. <i>Journal of Molecular Liquids</i> , 2015, 208, 322-332.	2.3	65
7358	Corrosion inhibition effect of pyrazole derivatives on mild steel in hydrochloric acid solution. <i>Journal of Adhesion Science and Technology</i> , 2015, 29, 1690-1713.	1.4	60

#	ARTICLE	IF	CITATIONS
7359	Mapping the genome of meta-generalized gradient approximation density functionals: The search for B97M-V. <i>Journal of Chemical Physics</i> , 2015, 142, 074111.	1.2	305
7360	Intersystem-crossing and phosphorescence rates in fac-Ir(ppy) ₃ : A theoretical study involving multi-reference configuration interaction wavefunctions. <i>Journal of Chemical Physics</i> , 2015, 142, 094301.	1.2	75
7361	Theoretical Study of Acene-Bridged Dyes for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3299-3309.	1.1	48
7362	Lithium and sodium storage on tetracyanoethylene (TCNE) and TCNE-(doped)-graphene complexes: A computational study. <i>Materials Chemistry and Physics</i> , 2015, 156, 180-187.	2.0	34
7363	Schiff base fluorescence probes for Cu ²⁺ based on imidazole and benzimidazole. <i>Sensors and Actuators B: Chemical</i> , 2015, 214, 138-143.	4.0	28
7364	Determination of thermodynamic properties for protonation equilibrium between isomeric cresols and N,N-dimethylaniline in n-hexane medium. <i>Journal of Molecular Liquids</i> , 2015, 207, 28-38.	2.3	6
7365	Comprehensive UV-Vis and EPR spectroelectrochemical characterization of ambipolar azomethinenaphthalidiimides. <i>Journal of Electroanalytical Chemistry</i> , 2015, 745, 14-21.	1.9	7
7366	Thiol-maleimide click-chemistry: evaluating the influence of solvent, initiator, and thiol on the reaction mechanism, kinetics, and selectivity. <i>Polymer Chemistry</i> , 2015, 6, 3415-3430.	1.9	154
7367	Theoretical Studies of Pendant Effects on the Properties of Sulfonated Hydrocarbon Polymer Electrolyte Membranes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11362-11369.	1.5	7
7368	Molybdenum-Catalyzed Conversion of Diols and Biomass-Derived Polyols to Alkenes Using Isopropyl Alcohol as Reductant and Solvent. <i>ACS Catalysis</i> , 2015, 5, 3638-3647.	5.5	78
7369	Effect of Sulfuric and Triflic Acids on the Hydration of Vanadium Cations: An <i>ab Initio</i> Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5749-5761.	1.1	29
7370	HO + OClO Reaction System: Featuring a Barrierless Entrance Channel with Two Transition States. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5723-5731.	1.1	20
7371	Electron Transport in Graphene-Based Nanosensors for Eu(III) Detection. <i>Journal of Physical Chemistry C</i> , 2015, 119, 12037-12046.	1.5	6
7372	Mechanistic Studies on the Switching from Ethylene Polymerization to Nonselective Oligomerization over the Triphenylsiloxy Chromium(II)/Methylaluminumoxane Catalyst. <i>ACS Catalysis</i> , 2015, 5, 3562-3574.	5.5	20
7373	Noble-Gas-Inserted Fluoro(sulphido)boron (FN _g BS, N _g = Ar, Kr, and Xe): A Theoretical Prediction. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5732-5741.	1.1	22
7374	Conformational Stability and Thermal Pathways of Relaxation in Triclosan (Antibacterial/Excipient/Contaminant) in Solid-State: Combined Spectroscopic (¹ H NMR) and Computational (Periodic DFT) Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4864-4874.	1.1	21
7375	Stereoselective Syntheses of (+)-2-epi-Deoxoprosopinine, (âˆ’)-Deoxoprosophylline, (+)-cis-195A, and 2,5-Di-epi-cis-195A from a Common Chiral Nonracemic Building Block. <i>Journal of Organic Chemistry</i> , 2015, 80, 5236-5251.	1.7	13
7376	Relative affinity of bambus[6]uril towards halide ions: A DFT/GIAO approach in the gas phase, and in the presence of the solvent employing discrete and discrete-continuum models. <i>Computational and Theoretical Chemistry</i> , 2015, 1064, 35-44.	1.1	6

#	ARTICLE	IF	CITATIONS
7377	Structural, Magnetic, and Redox Diversity of First-Row Transition Metal Complexes of a Pyridine-Based Macrocyclic: Well-Marked Trends Supported by Theoretical DFT Calculations. <i>Inorganic Chemistry</i> , 2015, 54, 3352-3369.	1.9	39
7378	Single Molecule Investigation of Glycine-Chlorite Interaction by Cross-Correlated Scanning Probe Microscopy and Quantum Mechanics Simulations. <i>Langmuir</i> , 2015, 31, 4453-4463.	1.6	21
7379	Surface Confined Retro Diels-Alder Reaction Driven by the Swelling of Weak Polyelectrolytes. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 6254-6259.	4.0	25
7380	Structure and Conformation of Protonated d-(+)-Biotin in the Unsolvated State. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6198-6203.	1.2	10
7381	Phenothiazine Decorated Carbazoles: Effect of Substitution Pattern on the Optical and Electroluminescent Characteristics. <i>Journal of Organic Chemistry</i> , 2015, 80, 5812-5823.	1.7	63
7382	Bond Dissociation Energies of C ₁₀ and C ₁₈ Methyl Esters from Local Multireference Averaged-Coupled Pair Functional Theory. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3429-3439.	1.1	27
7383	Photoinduced Energy Shift in Quantum-Dot-Sensitized TiO ₂ : A First-Principles Analysis. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1423-1429.	2.1	10
7384	The driving forces for twisted or planar intramolecular charge transfer. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9248-9257.	1.3	92
7385	Excited-state intramolecular proton transfer to carbon atoms: nonadiabatic surface-hopping dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9687-9697.	1.3	52
7386	Synthesis and Charge-Transfer Dynamics in a Ferrocene-Containing Organoboryl aza-BODIPY Donor-Acceptor Triad with Boron as the Hub. <i>Inorganic Chemistry</i> , 2015, 54, 4167-4174.	1.9	63
7387	Conformational Analysis and Electronic Interactions of Some 4-Substituted-2-ethylthio-phenylacetates. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3823-3832.	1.1	5
7388	Photoinduced Excited-State Energy-Transfer Dynamics of a Nitrogen-Cored Symmetric Dendrimer: From the Perspective of the Jahn-Teller Effect. <i>Journal of Physical Chemistry C</i> , 2015, 119, 7578-7589.	1.5	15
7389	Thermodynamic and quantum-chemical study of the oxidative dehydrogenation of ethane to ethylene. <i>Petroleum Chemistry</i> , 2015, 55, 146-153.	0.4	11
7390	Synthesis, crystal structure, antibacterial activity and theoretical studies on a novel mononuclear cobalt(II) complex based on 2,4,6-tris(2-pyridyl)-1,3,5-triazine ligand. <i>Journal of Molecular Structure</i> , 2015, 1093, 24-32.	1.8	32
7391	Design and synthesis of sugar-triazole based uracil appended sugar-imine derivatives – an application in DNA binding studies. <i>New Journal of Chemistry</i> , 2015, 39, 4575-4582.	1.4	9
7392	Comparison of Three Isoelectronic Multiple-Well Reaction Systems: OH + CH ₂ O, OH + CH ₂ CH ₂ , and OH + CH ₂ NH. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7578-7592.	1.1	47
7393	Second hyperpolarizability of multimetalloenes [<i>Cp</i> - <i>M</i> _n - <i>Cp</i>] of <i>Be</i> , <i>Mg</i> and <i>Ca</i> . <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550002.	1.8	7
7394	Origin of molecular conformational stability: Perspectives from molecular orbital interactions and density functional reactivity theory. <i>Journal of Chemical Physics</i> , 2015, 142, 054107.	1.2	57

#	ARTICLE	IF	CITATIONS
7395	Computational Investigation of Acene-Modified Zinc-Porphyrin Based Sensitizers for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2015, 119, 8417-8430.	1.5	22
7396	New trans-stilbene derivatives with large two-photon absorption cross-section and non-linear optical susceptibility values – a theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12299-12309.	1.3	4
7397	Feasibility of Intramolecular Proton Transfers in Terpene Biosynthesis – Guiding Principles. <i>Journal of the American Chemical Society</i> , 2015, 137, 4134-4140.	6.6	31
7398	Donor/Acceptor Indenoperylene Dye for Highly Efficient Organic Dye-Sensitized Solar Cells. <i>Journal of the American Chemical Society</i> , 2015, 137, 3799-3802.	6.6	528
7399	A new pentacoordinate polymeric copper(II) complex with 2-amino-2-methyl-1,3-propanediol: Structural investigations using XRD and DFT. <i>Journal of Structural Chemistry</i> , 2015, 56, 92-101.	0.3	7
7400	Conformation change of opiorphin derivatives. A theoretical study of the radical initiated epimerization of opiorphin. <i>Chemical Physics Letters</i> , 2015, 626, 29-38.	1.2	0
7401	A combined experimental and theoretical studies on FT-IR, FT-Raman and UV-vis spectra of 2-chloro-3-quinolinecarboxaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 148, 163-174.	2.0	23
7402	The Electrolyte Genome project: A big data approach in battery materials discovery. <i>Computational Materials Science</i> , 2015, 103, 56-67.	1.4	150
7403	Design and synthesis of fluorenone-based dyes: two-photon excited fluorescent probes for imaging of lysosomes and mitochondria in living cells. <i>Journal of Materials Chemistry B</i> , 2015, 3, 3315-3323.	2.9	50
7404	Understanding the Effects of Bidentate Directing Groups: A Unified Rationale for sp ² and sp ³ C-H Bond Activations. <i>Journal of Organic Chemistry</i> , 2015, 80, 4672-4682.	1.7	58
7405	Theoretical study of tautomeric equilibria of 2,6-diamino-8-azapurine and 8-aza-iso-Guanine. <i>Chemical Physics Letters</i> , 2015, 627, 30-35.	1.2	8
7406	Synthesis, structural characterization and theoretical approach of the tri(2-(2,6-dichlorophenyl)-1H-imidazo[4,5-f][1,10]phenanthroline) cobalt(II). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 147, 31-42.	2.0	5
7407	Electronic Structure of Ni ₂ E ₂ Complexes (E = S, Se, Te) and a Global Analysis of M ₂ E ₂ Compounds: A Case for Quantized E ₂ ⁺ Oxidation Levels with <i>n</i> = 2, 3, or 4. <i>Journal of the American Chemical Society</i> , 2015, 137, 4993-5011.	6.6	26
7408	New bipolar host materials for high performance of phosphorescent green organic light-emitting diodes. <i>RSC Advances</i> , 2015, 5, 31282-31291.	1.7	11
7409	Comparative Kinetics of the 3-Buten-1-ol and 1-Butene Reactions with OH Radicals: A Density Functional Theory/RRKM Investigation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3171-3180.	1.1	10
7410	Sequential palladium catalyzed coupling-cyclocondensation-coupling (C ³) four-component synthesis of intensively blue luminescent biarylsubstituted pyrazoles. <i>RSC Advances</i> , 2015, 5, 33838-33854.	1.7	32
7411	Novel 6-(1H-benzo[d]imidazol-2-yl) benzo[a]phenazin-5-ol Derivatives with Dual Emission and Large Stokes Shift Synthesis, Photophysical Properties and Computational Studies. <i>Journal of Fluorescence</i> , 2015, 25, 835-848.	1.3	2
7412	Identification and in silico prediction of metabolites of the model compound, tebufenozide by human CYP3A4 and CYP2C19. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 6594-6601.	1.4	2

#	ARTICLE	IF	CITATIONS
7413	ON THE ORIGIN OF THE 11.3 MICRON UNIDENTIFIED INFRARED EMISSION FEATURE. <i>Astrophysical Journal</i> , 2015, 807, 95.	1.6	20
7414	Benchmark thermochemistry of chloramines, bromamines, and bromochloramines: halogen oxidants stabilized by electron correlation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 3584-3598.	1.3	8
7415	Experimental and theoretical study of phase separation in ZnPc:C60 blends. <i>Organic Electronics</i> , 2015, 27, 183-191.	1.4	5
7416	Synthesis, structure, and reactivity of iridium perfluorocarbene complexes: regio- and stereo-specific addition of HCl across a metal carbon double bond. <i>Dalton Transactions</i> , 2015, 44, 19528-19542.	1.6	6
7417	Cation-Controlled Enantioselective and Diastereoselective Synthesis of Indolines: An Autoinductive Phase-Transfer Initiated 5-endo-trig Process. <i>Journal of the American Chemical Society</i> , 2015, 137, 13414-13424.	6.6	43
7418	Ionization and Fragmentation of Formamide Induced by Synchrotron Radiation in the Valence Region via Photoelectron Photoion Coincidence Measurements and Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10300-10308.	1.1	8
7419	Structural and spectral properties of tartrato complexes of vanadium(V) from quantum chemical calculations. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	0
7420	Impact of Aromatic Ring Count on the Ability to Participate in Attractive Interactions. Crystal Structure (X-ray) and Solid State Computational (DFT/QTAIM/RDS/Hirshfeld-surfaces) Study of 1,4-di(2-phenyl-1H-imidazol-4-yl)benzene. A Potential Nanotechnology Intrinsic Component. <i>Crystal Growth and Design</i> , 2015, 15, 5464-5475.	1.4	4
7421	Performance and Accuracy of Recursive Subspace Bisection for Hybrid DFT Calculations in Inhomogeneous Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4655-4663.	2.3	28
7422	Novel Iminocoumarin Derivatives: Synthesis, Spectroscopic and Computational Studies. <i>Journal of Fluorescence</i> , 2015, 25, 1615-1628.	1.3	18
7423	Geometry Optimization, Spectral Analysis, Molecular Electrostatic Potential Surface, and Nonlinear Optical Activity of 4-Methyl Anilinium Phenolsulfonate: a DFT Study. <i>Journal of Applied Spectroscopy</i> , 2015, 82, 687-699.	0.3	6
7424	Unravelling the interplay of dopant concentration and band structure engineering of monoclinic niobium pentoxide: A model photoanode for water splitting. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 13867-13875.	3.8	22
7425	NLOphoric studies in thiazole containing symmetrical push-pull fluorophores: Combined experimental and DFT approach. <i>Optical Materials</i> , 2015, 48, 271-280.	1.7	13
7426	The electronic structures and photophysical properties of platinum complexes with C ^N N ligands: the influence of the carborane substituent. <i>Dalton Transactions</i> , 2015, 44, 18130-18137.	1.6	28
7427	Impact of alkoxy chain length on carbazole-based, visible light-driven, dye sensitized photocatalytic hydrogen production. <i>Journal of Materials Chemistry A</i> , 2015, 3, 21713-21721.	5.2	33
7428	Insight into quinoxaline containing D-π-A dyes for dye-sensitized solar cells with cobalt and iodine based electrolytes: the effect of π-bridge on the HOMO energy level and photovoltaic performance. <i>Journal of Materials Chemistry A</i> , 2015, 3, 21733-21743.	5.2	47
7429	Excited State Studies of Polyacenes Using the All-Order Constricted Variational Density Functional Theory with Orbital Relaxation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10575-10581.	1.1	9
7430	Benchmarking Electronic Excitation Energies and Transitions in Peptide Radicals. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10101-10111.	1.1	24

#	ARTICLE	IF	CITATIONS
7431	Dynamic Characteristics of Aggregation Effects of Organic Dyes in Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 22504-22514.	4.0	39
7432	Low-Valent Iron Mono-Diazadiene Compounds: Electronic Structure and Catalytic Application. ACS Catalysis, 2015, 5, 6230-6240.	5.5	48
7433	Theoretical studies on the carrier tunability of oxidized oligothiophenes. Physical Chemistry Chemical Physics, 2015, 17, 26703-26709.	1.3	9
7434	Mechanistic insights into small molecule activation induced by ligand cooperativity in PCcarbeneP nickel pincer complexes: a quantum chemistry study. Journal of Molecular Modeling, 2015, 21, 242.	0.8	12
7435	H-atom loss and migration in hydrogen-rich peptide cation radicals: The role of chemical environment. International Journal of Mass Spectrometry, 2015, 390, 28-38.	0.7	7
7436	Sequence specific recognition of ssDNA by fluorophore 3-hydroxyflavone. Journal of Photochemistry and Photobiology B: Biology, 2015, 153, 391-396.	1.7	4
7437	Demystifying fluorine chemical shifts: electronic structure calculations address origins of seemingly anomalous ^{19}F -NMR spectra of fluorohistidine isomers and analogues. Physical Chemistry Chemical Physics, 2015, 17, 30606-30612.	1.3	22
7438	Atmospheric chemistry of alkyl iodides: theoretical studies on the mechanisms and kinetics of $\text{CH}_3\text{I}/\text{C}_2\text{H}_5\text{I} + \text{NO}_3$ reactions. RSC Advances, 2015, 5, 88087-88095.	1.7	13
7439	Tension between Internal and External Modes of Stabilization in Carbocations Relevant to Terpene Biosynthesis: Modulating Minima Depth via $\text{H}\cdots\text{H}\cdots\text{I}$ Interactions. Organic Letters, 2015, 17, 5388-5391.	2.4	22
7440	Stable Germenolates and Germenes with Exocyclic Structures. Organometallics, 2015, 34, 5291-5297.	1.1	24
7441	Critical Analysis of Cluster Models and Exchange-Correlation Functionals for Calculating Magnetic Shielding in Molecular Solids. Journal of Chemical Theory and Computation, 2015, 11, 5229-5241.	2.3	60
7442	Two-Step Synthesis of Blue Luminescent (Pyrrol-3-yl)-1 <i>H</i> -(<i>aza</i>)indazoles Based on a Three-Component Coupling-Cyclocondensation Sequence. European Journal of Organic Chemistry, 2015, 2015, 5128-5142.	1.2	8
7443	The structural, electronic, and optical properties of NpO_2 and PuO_2 : a hybrid density-functional-theory study. European Physical Journal B, 2015, 88, 1.	0.6	2
7444	Influence of Solvation and Structural Contributions on Fluorescence of Dipyrrine Dyes. Journal of Fluorescence, 2015, 25, 1875-1885.	1.3	4
7445	Ethylene adsorption and transformation on zeolite $\text{Ga}^+/\text{ZSM-5}$. Russian Chemical Bulletin, 2015, 64, 278-283.	0.4	2
7446	How Bonding in Manganous Phosphates Affects their $\text{Mn(II)}^{31}\text{P}$ Hyperfine Interactions. Inorganic Chemistry, 2015, 54, 10422-10428.	1.9	7
7447	Tuning the Reactivity of Chromium(III)-Superoxo Species by Coordinating Axial Ligands. Inorganic Chemistry, 2015, 54, 10513-10520.	1.9	21
7448	Electronic transport properties of thiol-ended Ge_4 , Sn_2Ge_2 , and Sn_4 nanoclusters: A DFT-NEGF study. Computational Materials Science, 2015, 110, 182-190.	1.4	2

#	ARTICLE	IF	CITATIONS
7449	Guanosine-based hydrogen-bonded 2D scaffolds: metal-free formation of G-quartet and G-ribbon architectures at the solid/liquid interface. <i>Chemical Communications</i> , 2015, 51, 11677-11680.	2.2	38
7450	One-Pot Domino Aldol Reaction of Indium Enolates Affording 6-Deoxy- β -D-altropyranose Derivatives: Synthesis, Mechanism, and Computational Results. <i>Journal of Organic Chemistry</i> , 2015, 80, 8175-8182.	1.7	12
7451	N ⁺ H Activation of Ammonia by $[M(\eta^4\text{-OMe})(\text{cod})]_2$ (M = Ir, Rh) Complexes: A DFT Study. <i>Organometallics</i> , 2015, 34, 3959-3966.	1.1	20
7452	Carbon-Atom Extrusion from Halobenzenes and Its Coupling with a Methylene Ligand to Form Acetylene. <i>Chemistry - A European Journal</i> , 2015, 21, 9629-9631.	1.7	12
7453	Density Functional Theory Study of Atomic Layer Deposition of Zinc Oxide on Graphene. <i>Nanoscale Research Letters</i> , 2015, 10, 1008.	3.1	6
7454	Corrosion inhibition effect of spiropyrimidinethiones on mild steel in 15% HCl solution: insight from electrochemical and quantum studies. <i>RSC Advances</i> , 2015, 5, 70832-70848.	1.7	102
7455	The electronic characterization of biphenylene—Experimental and theoretical insights from core and valence level spectroscopy. <i>Journal of Chemical Physics</i> , 2015, 142, 074305.	1.2	24
7456	Local hybrid functionals with orbital-free mixing functions and balanced elimination of self-interaction error. <i>Journal of Chemical Physics</i> , 2015, 142, 074112.	1.2	31
7457	Generic expansion of the Jastrow correlation factor in polynomials satisfying symmetry and cusp conditions. <i>Journal of Chemical Physics</i> , 2015, 142, 084111.	1.2	15
7458	A tight distance-dependent estimator for screening three-center Coulomb integrals over Gaussian basis functions. <i>Journal of Chemical Physics</i> , 2015, 142, 154106.	1.2	18
7459	Ensemble density functional theory method correctly describes bond dissociation, excited state electron transfer, and double excitations. <i>Journal of Chemical Physics</i> , 2015, 142, 184104.	1.2	40
7460	Spin Isomers and Ligand Isomerization in a Three-Coordinate Cobalt(I) Carbonyl Complex. <i>Journal of the American Chemical Society</i> , 2015, 137, 10689-10699.	6.6	25
7461	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. <i>Journal of Chemical Physics</i> , 2015, 143, 054107.	1.2	605
7462	Experimental and Theoretical Investigations of Magnetic Exchange Pathways in Structurally Diverse Iron(III) Schiff-Base Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 8625-8638.	1.9	35
7463	First principles-based multiparadigm, multiscale strategy for simulating complex materials processes with applications to amorphous SiC films. <i>Journal of Chemical Physics</i> , 2015, 142, 174703.	1.2	10
7464	Condensation pigments for pigment printing of cotton - synthesis, photophysical properties, TD-DFT studies. <i>Fibers and Polymers</i> , 2015, 16, 809-818.	1.1	1
7465	Field-induced slow relaxation of magnetization in a pentacoordinate Co(II) compound [Co(phen)(DMSO)Cl ₂]. <i>Dalton Transactions</i> , 2015, 44, 15014-15021.	1.6	40
7466	Homoleptic Transition Metal Complexes of the 7-Azaindolidine Ligand Featuring $\eta^1\text{-N1}$ Coordination. <i>Inorganic Chemistry</i> , 2015, 54, 9637-9645.	1.9	8

#	ARTICLE	IF	CITATIONS
7467	First-Principles Prediction of Enthalpies of Formation for Polycyclic Aromatic Hydrocarbons and Derivatives. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11329-11365.	1.1	38
7468	Thermal and Photolytic Transformation of NHC-B,N-Heterocycles: Controlled Generation of Blue Fluorescent 1,3-Azaborinine Derivatives and 1 <i>H</i> -imidazo[1,2- <i>e</i>]indoles by External Stimuli. <i>Chemistry - A European Journal</i> , 2015, 21, 13961-13970.	1.7	31
7469	Influence of the size and charge of gold nanoclusters on complexation with siRNA: a molecular dynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30307-30317.	1.3	12
7470	Why Ni is absent from the surface of La ₂ NiO ₄ + δ ?. <i>Journal of Materials Chemistry A</i> , 2015, 3, 23760-23767.	5.2	37
7471	Photo- and Thermal Isomerization of (TP)Fe(CO)Cl ₂ [TP = Bis(2-diphenylphosphinophenyl)phenylphosphine]. <i>Organometallics</i> , 2015, 34, 5009-5014.	1.1	9
7472	Vibrational relaxation as the driving force for wavelength conversion in the peridinin-chlorophyll <i>a</i> -protein. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2015, 1847, 1509-1517.	0.5	7
7473	Energetics and electronic structure of UAl ₄ with point defects. <i>Journal of Nuclear Materials</i> , 2015, 466, 539-550.	1.3	4
7474	Phase Transitions of Triflate-Based Ionic Liquids under High Pressure. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14315-14322.	1.2	19
7475	Reversible encapsulation in a covalent capsule. <i>Chemical Physics Letters</i> , 2015, 633, 99-104.	1.2	3
7476	Density functional theories study on the properties of Ga _{1-x} CrxAs. <i>Materials and Design</i> , 2015, 87, 877-882.	3.3	4
7477	Phenothiazine-based bipolar green-emitters containing benzimidazole units: synthesis, photophysical and electroluminescence properties. <i>RSC Advances</i> , 2015, 5, 87416-87428.	1.7	29
7478	Synthesis, structure and magnetic characterization of dinuclear copper(<i>II</i>) complexes bridged by bicompartamental phenolate. <i>RSC Advances</i> , 2015, 5, 87139-87150.	1.7	32
7479	Electronic Structure and Reactivity of a Well-Defined Mononuclear Complex of Ti(II). <i>Inorganic Chemistry</i> , 2015, 54, 10380-10397.	1.9	34
7480	Stereoisomeric Composition of Natural Myrtucommulone A. <i>Journal of Natural Products</i> , 2015, 78, 2381-2389.	1.5	21
7481	Quantum Chemical Study of the Thermochemical Properties of Organophosphorous Compounds. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10527-10539.	1.1	29
7482	Design Proposals for Organic Materials Exhibiting a Low Exciton Binding Energy. <i>Journal of Physical Chemistry C</i> , 2015, 119, 22820-22825.	1.5	38
7483	Theoretical description of efficiency enhancement in DSSCs sensitized by newly synthesized heteroleptic Ru complexes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29574-29585.	1.3	20
7484	Size-dependent properties of transition metal clusters: from molecules to crystals and surfaces - computational studies with the program ParaGauss. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28463-28483.	1.3	16

#	ARTICLE	IF	CITATIONS
7485	Chemical trends in the optical properties of rocksalt nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28892-28900.	1.3	10
7486	Ice chemistry of acetaldehyde reveals competitive reactions in the first step of the Strecker synthesis of alanine: formation of HO-CH(CH ₃)-NH ₂ vs. HO-CH(CH ₃)-CN. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 451, 1649-1660.	1.6	13
7487	Structure, solvent, and relativistic effects on the NMR chemical shifts in square-planar transition-metal complexes: assessment of DFT approaches. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24944-24955.	1.3	82
7488	Towards an understanding of the singlet-triplet splittings in conjugated hydrocarbons: azulene investigated by anion photoelectron spectroscopy and theoretical calculations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 23573-23581.	1.3	28
7489	Anti-aggregation and intra-type Förster resonance energy transfer in bulky indoline sensitizers for dye-sensitized solar cells: a combined DFT/TDDFT and molecular dynamics study. <i>Journal of Materials Chemistry A</i> , 2015, 3, 19948-19959.	5.2	16
7490	Partition, orientation and mobility of ubiquinones in a lipid bilayer. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2015, 1847, 1560-1573.	0.5	59
7491	Systematic Improvement of Density Functionals through Parameter-Free Hybridization Schemes. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3540-3545.	2.1	44
7492	Substrate-Assisted and Enzymatic Pretransfer Editing of Nonstandard Amino Acids by Methionyl-tRNA Synthetase. <i>Biochemistry</i> , 2015, 54, 5757-5765.	1.2	11
7493	Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to <i>K</i> -edge X-ray Absorption Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4146-4153.	2.3	92
7494	Mechanism of Metal-Free C-H Activation of Branched Aldehydes and Acylation of Alkenes Using Hypervalent Iodine Compound: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2015, 80, 9264-9271.	1.7	34
7495	Electronic structure and second hyperpolarizability of M(NA) ₂ (M = Be, Mg, Ca; A = H, Li, Na) complexes. <i>Chemical Physics Letters</i> , 2015, 637, 164-171.	1.2	11
7496	Efficient Semi-numerical Implementation of Global and Local Hybrid Functionals for Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4226-4237.	2.3	54
7497	Combined molecular dynamics and continuum solvent approaches (MM-PBSA/GBSA) to predict nospapinoid binding to β -tubulin dimer. <i>SAR and QSAR in Environmental Research</i> , 2015, 26, 507-519.	1.0	15
7498	Amino acid-type interactions of L-3,4-dihydroxyphenylalanine with transition metal ions: An experimental and theoretical investigation. <i>Journal of Molecular Structure</i> , 2015, 1100, 162-173.	1.8	10
7499	Paddlewheel 1,2,4-diazaphospholide dibismuthanes with very short bismuth-bismuth single bonds. <i>Chemical Communications</i> , 2015, 51, 16184-16187.	2.2	23
7500	Electronic excitations in molecular solids: bridging theory and experiment. <i>Faraday Discussions</i> , 2015, 177, 181-202.	1.6	11
7501	The reactivity of stoichiometric tungsten oxide clusters towards carbon monoxide: the effects of cluster sizes and charge states. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11499-11508.	1.3	7
7502	A one-pot dilithiation-lithium-zinc exchange-Negishi coupling approach to 2,6-di(hetero)aryl substituted dithienothiazines - a novel class of electronically fine-tunable redox systems. <i>Organic Chemistry Frontiers</i> , 2015, 2, 481-491.	2.3	9

#	ARTICLE	IF	CITATIONS
7503	On the relation between local and charge-transfer exciton binding energies in organic photovoltaic materials. Proceedings of SPIE, 2015, , .	0.8	0
7504	N-2-Aryl-1,2,3-Triazoles: A novel class of blue-green emitting fluorophores-synthesis, photophysical properties study and dft computations. Journal of Luminescence, 2015, 168, 114-123.	1.5	9
7505	Radical Mechanism of Isocyanide-Alkyne Cycloaddition by Multicatalysis of Ag ₂ CO ₃ , Solvent, and Substrate. ACS Catalysis, 2015, 5, 6177-6184.	5.5	54
7506	Phosphoryl transfer reaction catalyzed by membrane diacylglycerol kinase: a theoretical mechanism study. Physical Chemistry Chemical Physics, 2015, 17, 25228-25234.	1.3	1
7507	Efficient Pt(II) emitters assembled from neutral bipyridine and dianionic bipyrazolate: designs, photophysical characterization and the fabrication of non-doped OLEDs. Journal of Materials Chemistry C, 2015, 3, 10837-10847.	2.7	31
7508	On the photophysics of four heteroleptic iridium(III) phenylpyridyl complexes investigated by relativistic multi-configuration methods. Molecular Physics, 0, , 1-16.	0.8	13
7509	Critical test of some computational methods for prediction of NMR ¹ H and ¹³ C chemical shifts. Journal of Molecular Modeling, 2015, 21, 244.	0.8	30
7510	Collision-induced dissociation pathways of protonated Gly ₂ NH ₂ and Gly ₃ NH ₂ in the short time-scale limit by chemical dynamics and ion spectroscopy. International Journal of Mass Spectrometry, 2015, 388, 40-52.	0.7	34
7511	Proximal Pocket Hydrogen Bonds Significantly Influence the Mechanism of Chloroperoxidase Compound I Formation. Journal of Physical Chemistry B, 2015, 119, 12590-12602.	1.2	6
7512	Unusual bonding modes of perfluorobenzene in its polymeric (dimeric, trimeric and tetrameric) forms: entirely negative fluorine interacting cooperatively with entirely negative fluorine. Physical Chemistry Chemical Physics, 2015, 17, 31624-31645.	1.3	34
7513	The energetic viability of an unexpected skeletal rearrangement in cyclooctatin biosynthesis. Organic and Biomolecular Chemistry, 2015, 13, 10273-10278.	1.5	40
7514	The effect of (H ₂ O) _n (n=1-2) or H ₂ S on the hydrogen abstraction reaction of H ₂ S by OH radicals in the atmosphere. Computational and Theoretical Chemistry, 2015, 1069, 77-85.	1.1	25
7515	Simulating Cl K-edge X-ray absorption spectroscopy in MCl ₆ ²⁻ (M = U, Np, Pu) complexes and UOCl ₅ - using time-dependent density functional theory. Highlights in Theoretical Chemistry, 2015, , 247-253.	0.0	2
7516	Predicting hydration propensities of biologically relevant α -ketoamides. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4153-4157.	1.0	5
7517	On novel magnetic probe for fullerene characterization: Theoretical studies on NMR parameters of free and confined in fullerenes HD and H ₂ molecules. Journal of Molecular Graphics and Modelling, 2015, 62, 26-37.	1.3	8
7518	A systematic benchmark of the <i>ab initio</i> Bethe-Salpeter equation approach for low-lying optical excitations of small organic molecules. Journal of Chemical Physics, 2015, 142, 244101.	1.2	137
7519	Computational study on stereoselective synthesis of substituted 1H-tetrazoles via a click reaction: DFT and QTAIM approaches. Computational and Theoretical Chemistry, 2015, 1071, 53-60.	1.1	19
7520	Aggregation induced emission and mechanochromism in pyrenoidimidazoles. Journal of Materials Chemistry C, 2015, 3, 9981-9988.	2.7	92

#	ARTICLE	IF	CITATIONS
7521	Effect of the functionalized β -bridge on porphyrin sensitizers for dye-sensitized solar cells: an in-depth analysis of electronic structure, spectrum, excitation, and intramolecular electron transfer. <i>Journal of Materials Chemistry C</i> , 2015, 3, 10129-10139.	2.7	25
7522	Nitrogen-Containing Ionic Liquids: Biodegradation Studies and Utility in Base-Mediated Reactions. <i>Australian Journal of Chemistry</i> , 2015, 68, 849.	0.5	10
7523	Redox Noninnocence of the Bridge in Copper(II) Salophen and Bis(oxamato) Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 9013-9026.	1.9	38
7524	Thermal and mechanical stability, electronic structure and energetic properties of Pu-containing pyrochlores: La ₂ -Pu Zr ₂ O ₇ and La ₂ Zr ₂ -Pu O ₇ (O ²⁻ and Y ³⁺). <i>Journal of Nuclear Materials</i> , 2015, 466, 162-171. ^{1.3}	1.3	18
7525	Experimental and Theoretical Investigations of the Bromination of Phenols with \hat{I}^2 and \hat{I}^3 Aliphatic Substituents, including Rings. <i>Journal of Organic Chemistry</i> , 2015, 80, 9292-9296.	1.7	1
7526	Adsorption properties and inhibition of mild steel corrosion in 1 M HCl solution by some bipyrazolic derivatives: Experimental and theoretical investigations. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2015, 51, 873-884.	0.3	59
7527	The effect of fluorine substitution on the conformation and aromaticity of \hat{I} -6-fluoro arene chromium tricarbonyl complexes – Density functional insights. <i>Computational and Theoretical Chemistry</i> , 2015, 1069, 125-131.	1.1	11
7528	Ultraporous, Water Stable, and Breathing Zirconium-Based Metal-Organic Frameworks with ftw Topology. <i>Journal of the American Chemical Society</i> , 2015, 137, 13183-13190.	6.6	149
7529	Properties of noncovalent tetraphenylporphine ²⁻ dyads as studied by different long-range and dispersion-corrected DFT functionals. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27399-27408.	1.3	8
7530	Exploring the mechanism of isomerisation and water-migration in the water-complexes of amino-acid $\langle \text{scp} \rangle$ -proline: electrostatic potential and vibrational analysis. <i>RSC Advances</i> , 2015, 5, 82587-82604.	1.7	7
7531	Reactivity of Dimeric Tetrazirconium(IV) Wells-Dawson Polyoxometalate toward Dipeptide Hydrolysis Studied by a Combined Experimental and Density Functional Theory Approach. <i>Inorganic Chemistry</i> , 2015, 54, 11477-11492.	1.9	32
7532	Binuclear sandwich and multi-decker sandwich compounds of alkali and alkaline-earth metals: a quantum chemical study. <i>Russian Chemical Bulletin</i> , 2015, 64, 540-550.	0.4	3
7533	Multiple approach to model unpaired spin density effects in H-ZSM5 zeolite with extra-framework O atom: H-abstraction reaction from methane. <i>Computational and Theoretical Chemistry</i> , 2015, 1074, 9-18.	1.1	2
7534	Amino acid compounds as eco-friendly corrosion inhibitor for N80 steel in HCl solution: Electrochemical and theoretical approaches. <i>Journal of Molecular Liquids</i> , 2015, 212, 731-738.	2.3	76
7535	DFT studies on the activation of C-H bonds on V/P mixed oxides. <i>Chinese Journal of Catalysis</i> , 2015, 36, 1528-1534.	6.9	5
7536	7-Hydroxyflavone Revisited. 2. Substitution Effect on Spectral and Acid-Base Properties in the Ground and Excited States. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12672-12685.	1.1	9
7537	Exploring bridging effect on first hyperpolarizability. <i>RSC Advances</i> , 2015, 5, 103729-103738.	1.7	32
7538	Comparative study on the methods for predicting the reactive site of nucleophilic reaction. <i>Science China Chemistry</i> , 2015, 58, 1845-1852.	4.2	105

#	ARTICLE	IF	CITATIONS
7539	Adsorption and corrosion inhibitive properties of synthesized hydrazine compounds on N80 steel/hydrochloric acid interface: Electrochemical and DFT studies. <i>Journal of Molecular Liquids</i> , 2015, 212, 451-460.	2.3	20
7540	Application of new isonicotinamides as a corrosion inhibitor on mild steel in acidic medium: Electrochemical, SEM, EDX, AFM and DFT investigations. <i>Journal of Molecular Liquids</i> , 2015, 212, 686-698.	2.3	60
7541	Monomeric Chiral and Achiral Basket-Handle Porphyrins: Synthesis, Structural Features, and Arrested Tautomerism. <i>Journal of Organic Chemistry</i> , 2015, 80, 12359-12378.	1.7	14
7542	Toward the construction of parameter-free doubly hybrid density functionals. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 589-595.	1.0	22
7543	Cyclometalated Fe(II) Complexes as Sensitizers in Dye-Sensitized Solar Cells. <i>Inorganic Chemistry</i> , 2015, 54, 560-569.	1.9	78
7544	³ He NMR studies on helium-pyrrole, helium-indole, and helium-carbazole systems: a new tool for following chemistry of heterocyclic compounds. <i>Magnetic Resonance in Chemistry</i> , 2015, 53, 103-109.	1.1	9
7545	In search of the appropriate theoretically justified mixing coefficient in parameter-free hybrid functionals for computing the NMR parameters. <i>RSC Advances</i> , 2015, 5, 4737-4746.	1.7	12
7546	Deep-blue emitting pyrene-benzimidazole conjugates for solution processed organic light-emitting diodes. <i>RSC Advances</i> , 2015, 5, 8727-8738.	1.7	31
7547	Quantum Chemistry in Proton-Conductors. <i>Advances in Quantum Chemistry</i> , 2015, , 31-67.	0.4	15
7548	Synthesis, antifungal activity, and QSAR study of novel trichodermin derivatives. <i>Journal of Asian Natural Products Research</i> , 2015, 17, 47-55.	0.7	10
7549	Synthesis and properties of 1,3,5-tricarbazolylbenzenes with star-shaped architecture. <i>Dyes and Pigments</i> , 2015, 113, 640-648.	2.0	15
7550	NIR-Emitting Boradiazaindacene Fluorophores -TD-DFT Studies on Electronic Structure and Photophysical Properties. <i>Journal of Fluorescence</i> , 2015, 25, 69-78.	1.3	23
7551	Rational design of biaryl pharmacophore inserted noscapine derivatives as potent tubulin binding anticancer agents. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 249-270.	1.3	35
7552	A Promising Candidate with D _{3h} Architecture as an Efficient Sensitizer for Dye-Sensitized Solar Cells. <i>ChemPhysChem</i> , 2015, 16, 601-606.	1.0	11
7553	An assessment of theoretical procedures for π -conjugation stabilisation energies in enones. <i>Molecular Physics</i> , 2015, 113, 1284-1296.	0.8	19
7554	Computational Analysis of the Stereochemical Outcome in the Imidazolidinone-Catalyzed Enantioselective (4 + 3)-Cycloaddition Reaction. <i>Journal of Organic Chemistry</i> , 2015, 80, 744-750.	1.7	26
7555	A Combined Experiment and Computation Study of the Fused Polycyclic Benzimidazole Derivatives. <i>Journal of Fluorescence</i> , 2015, 25, 127-136.	1.3	1
7556	Ambient-Stable, Annealing-Free, and Ambipolar Organic Field-Effect Transistors Based on Solution-Processable Poly(2,2-bis(trifluoromethyl)biphenyl-5,5'-divinylthiophene) without Long Alkyl Side Chains. <i>Advanced Functional Materials</i> , 2015, 25, 606-614.	7.8	17

#	ARTICLE	IF	CITATIONS
7557	Including Thermal Disorder of Hydrogen Bonding to Describe the Vibrational Circular Dichroism Spectrum of Zwitterionic α -Alanine in Water. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5099-5106.	1.1	6
7558	A Combined Experimental and Computational Investigation on the Unusual Molecular Mechanism of the Lossen Rearrangement Reaction Activated by Carcinogenic Halogenated Quinones. <i>Journal of Organic Chemistry</i> , 2015, 80, 180-189.	1.7	24
7559	Double Hybrid Functionals and the \hat{I} -System Bond Length Alternation Challenge: Rivaling Accuracy of Post-HF Methods. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 832-838.	2.3	22
7560	Kinetic and thermodynamical analysis of the reactivity of thiourea by association to Ca^{2+} . <i>Computational and Theoretical Chemistry</i> , 2015, 1052, 68-72.	1.1	1
7561	Intramolecular cyclization of \hat{I}^2 -nitroso- <i>o</i> -quinone methides. A theoretical endoscopy of a potentially useful innate α -reclusive reaction. <i>Tetrahedron</i> , 2015, 71, 359-369.	1.0	17
7562	Electron-Acceptor-Dependent Light Absorption and Charge-Transfer Dynamics in <i>N</i> -Annulated Perylene Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2015, 119, 980-988.	1.5	38
7563	Breaking bonds with electrons: stepwise and concerted reductive cleavage of C=S, C=Se and Se=CN bonds in phenacylthiocyanates and phenacylselenocyanates. <i>RSC Advances</i> , 2015, 5, 11753-11760.	1.7	15
7564	Theoretical study and design of multifunctional phosphorescent platinum(II) complexes containing triarylboron moieties for efficient OLED emitters. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2438-2446.	1.3	30
7565	Non-parametrized functionals with empirical dispersion corrections: A happy match?. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	16
7566	Theoretical investigation on atmospheric reaction of atomic O(3P) with acrylonitrile. <i>Computational and Theoretical Chemistry</i> , 2015, 1052, 17-25.	1.1	3
7567	Visualizing phosphodiester-bond hydrolysis by an endonuclease. <i>Nature Structural and Molecular Biology</i> , 2015, 22, 65-72.	3.6	30
7568	Ca K-Edge XAS as a Probe of Calcium Centers in Complex Systems. <i>Inorganic Chemistry</i> , 2015, 54, 1283-1292.	1.9	39
7569	Analytical Double-Hybrid Density Functional Based on the Polynomial Series Expansion of Adiabatic Connection: A Quadratic Approximation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 45-54.	2.3	22
7570	A DFT investigation on the electronic properties of octahaloditechnetate anions: Correlation between charge and bond strength. <i>Inorganica Chimica Acta</i> , 2015, 424, 308-315.	1.2	4
7571	Stabilization of a W ²⁶⁺ bimetallic complex supported by two N,N ⁺ ,N ³⁺ -triphenylguanidinate ligands. <i>Inorganica Chimica Acta</i> , 2015, 424, 286-292.	1.2	4
7572	DFT investigation on CO sensing characteristics of hexagonal and orthorhombic WO ₃ nanostructures. <i>Superlattices and Microstructures</i> , 2015, 78, 22-39.	1.4	34
7573	Total Synthesis of (\hat{A}) \hat{A} Hippolachnin \hat{A} ...A. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 2378-2382.	7.2	88
7574	Solvatochromism of BODIPY-Schiff Dye. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2576-2584.	1.2	37

#	ARTICLE	IF	CITATIONS
7575	Magnetic and structural properties of dinuclear singly bridged-phenoxido metal(μ_2) complexes. Dalton Transactions, 2015, 44, 2110-2121.	1.6	39
7576	Asymmetric Synthesis of Hydroxy Esters with Multiple Stereocenters via a Chiral Phosphoric Acid Catalyzed Kinetic Resolution. Journal of Organic Chemistry, 2015, 80, 133-140.	1.7	13
7577	Influence of oxygen nonstoichiometry and doping with 2p-, 3p-, 6p- and 3d-elements on electronic structure, optical properties and photocatalytic activity of rutile and anatase: Ab initio approaches. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2015, 22, 58-83.	5.6	28
7578	Assessment of various density functionals for intermolecular N \cdots Sn interactions: The test case of poly(trimethyltin cyanide). Computational and Theoretical Chemistry, 2015, 1051, 110-122.	1.1	12
7579	Electronic and optical properties of BBi and AlBi: Hybrid (YS-PBE0) function. Computational Materials Science, 2015, 98, 136-141.	1.4	25
7580	Computational insights into function and inhibition of fatty acid amide hydrolase. European Journal of Medicinal Chemistry, 2015, 91, 15-26.	2.6	40
7581	A combined magnetic circular dichroism and density functional theory approach for the elucidation of electronic structure and bonding in three- and four-coordinate iron(μ_2)-N-heterocyclic carbene complexes. Chemical Science, 2015, 6, 1178-1188.	3.7	44
7582	Theoretical studies on the effect of a bithiophene bridge with different substituent groups (R = H,) applications. Physical Chemistry Chemical Physics, 2015, 17, 2043-2053.	1.3	29
7583	Theoretical analysis of excited states and energy transfer mechanism in conjugated dendrimers. Journal of Computational Chemistry, 2015, 36, 151-163.	1.5	26
7584	Models of charge pair generation in organic solar cells. Physical Chemistry Chemical Physics, 2015, 17, 2311-2325.	1.3	158
7585	Accurate Ab Initio Description of Adsorption on Coordinatively Unsaturated Cu $^{2+}$ and Fe $^{3+}$ Sites in MOFs. Journal of Chemical Theory and Computation, 2015, 11, 230-238.	2.3	36
7586	DFT calculations and experimental FT-IR, FT-Raman, NMR, UV-Vis spectral studies of 3-fluorophenylboronic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 306-320.	2.0	33
7587	Competitive hydrogen atom migrations accompanying cascade dissociations of peptide cation-radicals of the + type. International Journal of Mass Spectrometry, 2015, 377, 44-53.	0.7	12
7588	Mechanisms of chromate adsorption on boehmite. Journal of Hazardous Materials, 2015, 281, 56-63.	6.5	40
7589	Theoretical Prediction of Noble Gas Inserted Thioformyl Cations: HN \cdots CS $^+$ (Ng = He, Ne, Ar,) Tj ETQq0 0.0 rgBT /Overlock 10	1.1	45
7590	On the multiple BO bonding using the topological analysis of Electron Localisation Function (ELF). Computational and Theoretical Chemistry, 2015, 1053, 130-141.	1.1	13
7591	Coumarin-bearing triarylamine sensitizers with high molar extinction coefficient for dye-sensitized solar cells. Journal of Power Sources, 2015, 273, 831-838.	4.0	47
7592	Anatomy of an iron-sulfur cluster scaffold protein: Understanding the determinants of [2Fe \cdots 2S] cluster stability on IscU. Biochimica Et Biophysica Acta - Molecular Cell Research, 2015, 1853, 1448-1456.	1.9	26

#	ARTICLE	IF	CITATIONS
7593	The importance of molecular conformation to the properties: a DFT study of the polynitro heterocyclic compounds based on dodecahydrodiimidazo [4,5-b:4'5'-e]pyrazine structure. <i>Structural Chemistry</i> , 2015, 26, 667-674.	1.0	3
7594	Novel dipolar 5,5,10,10-tetraphenyl-5,10-dihydroindeno[2,1-a]-indene derivatives for SM-OPV: A combined theoretical and experimental study. <i>Organic Electronics</i> , 2015, 16, 54-70.	1.4	9
7595	Calculating accurate barriers for olefin insertion and related reactions. <i>Journal of Organometallic Chemistry</i> , 2015, 775, 39-49.	0.8	56
7596	An unsymmetrical ferrocene based azine and its Cu(II) complex: Spectroscopy, crystal structure, electrochemistry and DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2015, 775, 80-87.	0.8	17
7597	A combined experimental and quantum mechanical investigation on some selected metal complexes of l-serine with first row transition metal cations. <i>Journal of Molecular Structure</i> , 2015, 1081, 281-292.	1.8	6
7598	œTschitschibabin type biradicals: benzenoid or quinoid?. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 983-991.	1.3	57
7599	First principles study of structural, electronic and magnetic properties of ferromagnetic Bi ₂ Fe ₄ O ₉ . <i>Journal of Alloys and Compounds</i> , 2015, 624, 131-136.	2.8	32
7600	Theoretical investigation on a series of novel S,S-dioxide diarylethenes with abnormal photochromic properties and design of new dyads. <i>New Journal of Chemistry</i> , 2015, 39, 1634-1642.	1.4	12
7601	A computational study of binding between 3-(4-fluorophenyl)-N-((4-fluorophenyl)sulphonyl)acrylamide and tubulin. <i>Molecular Simulation</i> , 2015, 41, 356-364.	0.9	2
7602	Effect of the anchoring group in the performance of carbazole-phenothiazine dyads for dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2015, 113, 536-545.	2.0	30
7603	Synthesis, optical, electrochemical and photovoltaic properties of organic dyes containing trifluorenylamine donors. <i>Dyes and Pigments</i> , 2015, 113, 78-86.	2.0	20
7604	Identification of potent inhibitors against snake venom metalloproteinase (SVMP) using molecular docking and molecular dynamics studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 1516-1527.	2.0	18
7605	Geometrical, electronic, and magnetic properties of Cu _n Fe (n=1-12) clusters: A density functional study. <i>Journal of Physics and Chemistry of Solids</i> , 2015, 76, 10-16.	1.9	26
7606	Photophysical properties of ESIPT inspired fluorescent 2-(2-hydroxyphenyl)-6-methylimidazo[4,5-f]isoindole-5,7(1H,6H)-dione and its derivative: Experimental and DFT based approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 135, 457-465.	2.0	14
7607	Linear response function of the Mayer bond order: an indicator to describe intrinsic chemical reactivity of molecules. <i>Molecular Physics</i> , 2015, 113, 336-341.	0.8	5
7608	Molecular Orbital Based Design Guideline for Hypergolic Ionic Liquids. <i>Propellants, Explosives, Pyrotechnics</i> , 2015, 40, 144-149.	1.0	15
7609	An experimental and TD-DFT theoretical study on the photophysical properties of Methylene Violet Bernthsen. <i>Dyes and Pigments</i> , 2015, 112, 341-351.	2.0	16
7610	Near-infrared absorbing isoindigo sensitizers: Synthesis and performance for dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2015, 112, 327-334.	2.0	42

#	ARTICLE	IF	CITATIONS
7611	Triphenylamine-functionalized corrole sensitizers for solar-cell applications. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2015, 212, 194-202.	0.8	26
7612	Insights into aggregation effects on optical property and electronic coupling of organic dyes in dye sensitized solar cells. <i>Journal of Power Sources</i> , 2015, 273, 282-289.	4.0	40
7613	Theoretical studies of electronic and optical properties of the triphenylamine-based organic dyes with diketopyrrolopyrrole chromophore. <i>Dyes and Pigments</i> , 2015, 113, 87-95.	2.0	50
7614	Synthesis, structure and spectral properties of dithiocarbamate bridged dirhenium(III,II) complexes: A combined experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2015, 424, 129-135.	1.2	13
7615	New mixed ligand oxorhenium(V) complexes of 3-thiapentane-1,5-dithiolato with 2-thiocytosine and 5-amino-1,3,4-thiadiazole-2-thiol: Experiment and theory. <i>Inorganica Chimica Acta</i> , 2015, 425, 124-133.	1.2	15
7616	Chemiluminescence properties of luminol related o-hydroxybenzimidazole analogues: Experimental and DFT based approach to photophysical properties. <i>Dyes and Pigments</i> , 2015, 113, 189-199.	2.0	9
7617	Synthesis and Photophysical Behavior of a Supramolecular Nanowire made from Dithienylethene-bridged Bis(permethyl- β -cyclodextrin)s and Porphyrins. <i>Chemistry - an Asian Journal</i> , 2015, 10, 84-90.	1.7	15
7618	QM/MM methodology, docking and spectroscopic (FT-IR/FT-Raman, NMR, UV) and Fukui function analysis on adrenergic agonist. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 841-855.	2.0	16
7619	Frequency and Zero-Point Vibrational Energy Scale Factors for Double-Hybrid Density Functionals (and Other Selected Methods): Can Anharmonic Force Fields Be Avoided?. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1701-1714.	1.1	441
7620	Derivative Couplings between Time-Dependent Density Functional Theory Excited States in the Random-Phase Approximation Based on Pseudo-Wavefunctions: Behavior around Conical Intersections. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7150-7161.	1.2	46
7621	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
7622	Molecular Level Factors Affecting the Efficiency of Organic Chromophores for p-Type Dye Sensitized Solar Cells. <i>Energies</i> , 2016, 9, 33.	1.6	14
7623	Effects of G-Quadruplex Topology on Electronic Transfer Integrals. <i>Nanomaterials</i> , 2016, 6, 184.	1.9	10
7624	Dynamic behavior of rearranging carbocations – implications for terpene biosynthesis. <i>Beilstein Journal of Organic Chemistry</i> , 2016, 12, 377-390.	1.3	79
7625	A density functional calculation on W doped Nn ($n=9$) clusters. <i>Main Group Chemistry</i> , 2016, 15, 243-256.	0.4	6
7626	Experimental and theoretical investigation of the reaction between CO ₂ and carbon dioxide binding organic liquids. <i>Turkish Journal of Chemistry</i> , 2016, 40, 706-719.	0.5	4
7627	Scope and mechanism of the highly stereoselective metal-mediated domino aldol reactions of enolates with aldehydes. <i>Beilstein Journal of Organic Chemistry</i> , 2016, 12, 813-824.	1.3	5
7628	The Iridoid Myodesert-1-ene and Elemol/Eudesmol are found in Distinct Chemotypes of the Australian Aboriginal Medicinal Plant <i>Eremophila dalyana</i> (Scrophulariaceae). <i>Natural Product Communications</i> , 2016, 11, 1934578X1601100.	0.2	8

#	ARTICLE	IF	CITATIONS
7629	Electronic structure of magnetic impurities and defects in semiconductors. , 2016, , 43-101.		5
7630	An Investigation of the Enolization and Isomeric Products Distribution in the Water Promoted Aldol Reaction of Tropinone and Granatanone. Journal of Chemistry, 2016, 2016, 1-15.	0.9	3
7632	The hydrolysis of geminal ethers: a kinetic appraisal of orthoesters and ketals. Beilstein Journal of Organic Chemistry, 2016, 12, 1467-1475.	1.3	7
7633	Combined experimental and theoretical studies of regio- and stereoselectivity in reactions of \hat{I}^2 -isoxazolyl- and \hat{I}^2 -imidazolyl enamines with nitrile oxides. Beilstein Journal of Organic Chemistry, 2016, 12, 2390-2401.	1.3	6
7634	Inhibition of DNA Topoisomerase Type II<i> \hat{I}^{\pm} <td>0.9</td> <td>21</td>	0.9	21
7635	The Influence of One-Electron Self-Interaction on d-Electrons. Computation, 2016, 4, 33.	1.0	12
7636	The Role of Coulomb Interactions for Spin Crossover Behaviors and Crystal Structural Transformation in Novel Anionic Fe(III) Complexes from a \hat{I}^{\pm} -Extended ONO Ligand. Crystals, 2016, 6, 49.	1.0	15
7637	Comparisons between Crystallography Data and Theoretical Parameters and the Formation of Intramolecular Hydrogen Bonds: Benznidazole. Crystals, 2016, 6, 56.	1.0	4
7638	Porphyrin Cobalt(III) \hat{I}^{\pm} -Nitrene Radical \hat{I}^{\pm} -Reactivity; Hydrogen Atom Transfer from Ortho-YH Substituents to the Nitrene Moiety of Cobalt-Bound Aryl Nitrene Intermediates (Y = O, NH). Molecules, 2016, 21, 242.	1.7	22
7639	Excited-State Proton Transfer and Decay in Hydrogen-Bonded Oxazole System: MS-CASPT2//CASSCF Study. Chinese Journal of Chemical Physics, 2016, 29, 38-46.	0.6	8
7640	Theoretical investigations of tautomeric equilibrium of 9-methyl-8-aza-iso-Guanine and its electrostatic properties. Computational and Theoretical Chemistry, 2016, 1091, 1-7.	1.1	4
7641	Intermolecular interactions in multi-component crystals of acridinone/thioacridinone derivatives: Structural and energetics investigations. Journal of Molecular Structure, 2016, 1125, 36-46.	1.8	3
7642	One-Pot Coupling \hat{I}^{\pm} -Coupling \hat{I}^{\pm} -Cyclocondensation Synthesis of Fluorescent Pyrazoles. Journal of Organic Chemistry, 2016, 81, 10328-10338.	1.7	42
7643	Novel aldehyde and thiosemicarbazone derivatives: Synthesis, spectroscopic characterization, structural studies and molecular docking studies. Journal of Molecular Structure, 2016, 1125, 470-480.	1.8	2
7644	Preparation of Imidazol \hat{I}^{\pm} -Cylidene Carbene Palladacycles with Bi \hat{I}^{\pm} - and Tridentate Schiff Bases \hat{I}^{\pm} Analyses of the Spectroscopic, Molecular Structure, and DFT Calculation Data. European Journal of Inorganic Chemistry, 2016, 2016, 422-431.	1.0	4
7645	From oxide to proton conduction: A quantum \hat{I}^{\pm} -chemical perspective on the versatility of Sr₂Fe_{1.5}Mo_{0.5}O₆ \hat{I}^{\pm} -based materials. International Journal of Quantum Chemistry, 2016, 116, 1501-1506.	1.0	13
7646	Experimental and theoretical investigation of the enantioselective hydrogenation of ethyl pyruvate with a Pt catalyst with new non-cinchona chiral modifiers. Journal of Molecular Catalysis A, 2016, 423, 233-239.	4.8	2
7647	Molecular Origin of the Charge Carrier Mobility in Small Molecule Organic Semiconductors. Advanced Functional Materials, 2016, 26, 5757-5763.	7.8	78

#	ARTICLE	IF	CITATIONS
7648	Spontaneous Formation of an Air-Stable Radical upon the Direct Fusion of Diphenylmethane to a Triarylporphyrin. <i>Angewandte Chemie</i> , 2016, 128, 8853-8856.	1.6	36
7649	Spontaneous Formation of an Air-Stable Radical upon the Direct Fusion of Diphenylmethane to a Triarylporphyrin. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8711-8714.	7.2	53
7650	Synthesis, Optical Properties, and Electronic Structures of Tetrakis(pentafluorophenyl)tetrathiaisophlorin Dioxide. <i>Chemistry - A European Journal</i> , 2016, 22, 9190-9197.	1.7	10
7651	Excited-State Intramolecular Proton Transfer in a Blue Fluorescence Chromophore Induces Dual Emission. <i>ChemPhysChem</i> , 2016, 17, 2340-2347.	1.0	27
7652	Cobalt(I) and Nickel(II) Complexes of Bis(1,3-diphosphacyclobutadiene) Sandwich Anions. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 736-742.	1.0	14
7653	The Spectroscopic Features of Ionized Water Medium: Theoretical Characterization and Implication Using $(\text{H}_2\text{O})_n^+$, $n=3-4$, Cluster Model. <i>Journal of the Chinese Chemical Society</i> , 2016, 63, 488-498.	0.8	3
7654	A novel organotriphosphoryl polyoxomolybdate: Synthesis, crystal structure, and experimental and theoretical investigation of the absorption spectra. <i>Inorganic Chemistry Communication</i> , 2016, 71, 15-18.	1.8	0
7655	Achieving high performance non-fullerene organic solar cells through tuning the numbers of electron deficient building blocks of molecular acceptors. <i>Journal of Power Sources</i> , 2016, 324, 538-546.	4.0	38
7656	Substituent effects on the ring-opening mechanism of gem-dibromospiropentanes to related allenes: a theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2016, 29, 63-68.	0.9	2
7657	Comparative Computational Studies of Gaseous Alkali Metal Amidoboranes $\text{M}(\text{NH}_2)_2\text{BH}_3$ and their Carbon Analogs $\text{M}(\text{C}_2\text{H}_5)_2\text{H}_5$ ($\text{M} = \text{Li}, \text{Cs}$): Formation and Unimolecular Hydrogen Evolution. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2016, 642, 163-168.	0.6	2
7658	Highly Active Palladium-Based Catalyst System for the Aerobic Oxidative Direct Coupling of Benzene to Biphenyl. <i>ChemCatChem</i> , 2016, 8, 448-454.	1.8	16
7659	A Combined Catalyst of Pt Nanoparticles and TiO_2 with Water-Tolerant Lewis Acid Sites for One-Pot Conversion of Glycerol to Lactic Acid. <i>ChemCatChem</i> , 2016, 8, 1094-1099.	1.8	49
7660	Rhodium-Catalyzed Intramolecular [5+2] Cycloaddition of Inverted 3-Acyloxy-1,4-dienyne and Alkyne: Experimental and Theoretical Studies. <i>Chemistry - A European Journal</i> , 2016, 22, 7079-7083.	1.7	13
7661	Bay-Annulated Perylene Tetraesters: A New Class of Discotic Liquid Crystals. <i>ChemPhysChem</i> , 2016, 17, 859-872.	1.0	30
7662	Mono-, Di-, and Polymeric Pyridino-ylhydrazone Zn^{II} Complexes: Structure and Photoluminescent Properties. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 818-825.	1.0	34
7663	Mechanism of Ylide Transfer to Carbonyl Compounds: Density Functional Calculations. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 830-839.	1.2	3
7664	Synthesis and Structural Characterization of Magnesium-Substituted Polystibides $[(\text{LMg})_4\text{Sb}_8]$. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4204-4209.	7.2	30
7665	Synthesis and Structural Characterization of Magnesium-Substituted Polystibides $[(\text{LMg})_4\text{Sb}_8]$. <i>Angewandte Chemie</i> , 2016, 128, 4276-4281.	1.6	19

#	ARTICLE	IF	CITATIONS
7666	Coordination contributions to protein stability in metal-substituted carbonic anhydrase. <i>Journal of Biological Inorganic Chemistry</i> , 2016, 21, 659-667.	1.1	16
7667	Tuning the push-pull configuration for efficient second-order nonlinear optical properties in some chalcone derivatives. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 68, 95-105.	1.3	77
7668	Efficient Ni ^{II} Ln ^{III} Electrocyclization Catalysts for the Synthesis of <i>trans</i> -4,5-Diaminocyclopent-2-enones from 2-Furaldehyde and Primary or Secondary Amines. <i>Inorganic Chemistry</i> , 2016, 55, 6988-6994.	1.9	55
7669	High Absorption Coefficient Cyclopentadithiophene Donor-Free Dyes for Liquid and Solid-State Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2016, 120, 15027-15034.	1.5	28
7670	Like Charges Attract?. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2689-2695.	2.1	26
7671	Superexchange Charge Transport in Loaded Metal Organic Frameworks. <i>ACS Nano</i> , 2016, 10, 7085-7093.	7.3	62
7672	Theoretical studies of the function switch and mechanism of AceK as a highly active ATPase. <i>RSC Advances</i> , 2016, 6, 68120-68127.	1.7	1
7673	Excited-State Dipole and Quadrupole Moments: TD-DFT versus CC2. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3993-4003.	2.3	41
7674	Ultrafast Intramolecular Photoinduced Energy Transfer Events in Benzothiazole-Borondipyrromethene Donor-Acceptor Dyads. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16305-16321.	1.5	22
7676	Cysteine Radical/Metal Ion Adducts: A Gas-Phase Structural Elucidation and Reactivity Study. <i>ChemPlusChem</i> , 2016, 81, 444-452.	1.3	8
7677	A Computational Approach to Predicting Ligand Selectivity for the Size-Based Separation of Trivalent Lanthanides. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 3474-3479.	1.0	31
7678	Comparative Computational Study of Hydrogen Abstraction Reactions of CY ₃ H + XO (X, Y = F, Cl, and) Tj ETQq _{1,1} 0.784314 rgBT (0.4)	0.4	0.784314
7679	Phenylene-Bridged Core-Modified Planar Aromatic Octaphyrin: Aromaticity, Photophysical and Anion Receptor Properties. <i>Chemistry - an Asian Journal</i> , 2016, 11, 1447-1453.	1.7	13
7680	Cascade Synthesis of Five-Membered Lactones using Biomass-Derived Sugars as Carbon Nucleophiles. <i>Chemistry - an Asian Journal</i> , 2016, 11, 1731-1737.	1.7	8
7681	Mechanistic Aspects of the Holmium-Mediated, Reciprocal Hydrogen/Sulfur Exchange in the Gas Phase: C ₆ H ₅ CH ₃ +CH ₂ S†C ₆ H ₅ CH ₃ +CH ₄ . <i>Chemistry - A European Journal</i> , 2016, 22, 4336-4339.		
7682	5-Substituted Benzothiophenes: Synthesis, Mechanism, and Kinetic Studies. <i>Helvetica Chimica Acta</i> , 2016, 99, 384-392.	1.0	6
7683	Evolution of DFT studies in view of a scientometric perspective. <i>Journal of Cheminformatics</i> , 2016, 8, 52.	2.8	31
7684	EPR Study of UV-Irradiated Thymidine Microcrystals Supports Radical Intermediates in Spore Photoproduct Formation. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10923-10931.	1.2	3

#	ARTICLE	IF	CITATIONS
7685	Ab-initio investigation of the influence of chemical compounds on graphene layer properties in fabricated IR detector. , 2016, , .		1
7686	Quantifying local exciton, charge resonance, and multiexciton character in correlated wave functions of multichromophoric systems. <i>Journal of Chemical Physics</i> , 2016, 144, 014102.	1.2	30
7687	Hydration effects on the electronic properties of eumelanin building blocks. <i>Journal of Chemical Physics</i> , 2016, 145, 084501.	1.2	14
7688	Promising Tools in Prostate Cancer Research: Selective Non-Steroidal Cytochrome P450 17A1 Inhibitors. <i>Scientific Reports</i> , 2016, 6, 29468.	1.6	43
7689	Conformational Dynamics and Protein-Substrate Interaction of ABC Transporter BtuCD at the Occluded State Revealed by Molecular Dynamics Simulations. <i>Biochemistry</i> , 2016, 55, 6897-6907.	1.2	9
7690	Analysis of the antioxidant activity of 4-(5-chloro-2-hydroxyphenylamino)-4-oxobut-2-enoic acid derivatives using quantum-chemistry descriptors and molecular docking. <i>Journal of Molecular Modeling</i> , 2016, 22, 302.	0.8	8
7691	Assessing the Accuracy of Across-the-Scale Methods for Predicting Carbohydrate Conformational Energies for the Examples of Glucose and α -Maltose. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6157-6168.	2.3	91
7692	Hartree potential dependent exchange functional. <i>Journal of Chemical Physics</i> , 2016, 145, 084110.	1.2	15
7693	Ultrafast electron and hole transfer in bulk heterojunctions of low-bandgap polymers. <i>Organic Photonics and Photovoltaics</i> , 2016, 4, .	1.3	7
7694	Redesign of the DFT/MRCI Hamiltonian. <i>Journal of Chemical Physics</i> , 2016, 144, 034104.	1.2	99
7695	Matrix effects in the C 1s photoabsorption spectra of condensed naphthalene. <i>Journal of Chemical Physics</i> , 2016, 145, 234307.	1.2	4
7696	Random phase approximation with second-order screened exchange for current-carrying atomic states. <i>Journal of Chemical Physics</i> , 2016, 145, 224106.	1.2	10
7697	SCAN-based hybrid and double-hybrid density functionals from models without fitted parameters. <i>Journal of Chemical Physics</i> , 2016, 144, 044114.	1.2	126
7698	Tuning the charge states of CrW2O9 clusters deposited on perfect and defective MgO(001) surfaces with different color centers: A comprehensive DFT study. <i>Journal of Chemical Physics</i> , 2016, 144, 174706.	1.2	4
7699	Could the description on polynuclear superhalogens by DFT be comparable with high-level <i>ab initio</i> results? A comparison between DFT and CCSD(T). <i>Journal of Chemical Physics</i> , 2016, 144, 054303.	1.2	19
7700	THE 6 μ m FEATURE AS A TRACER OF ALIPHATIC COMPONENTS OF INTERSTELLAR CARBONACEOUS GRAINS. <i>Astrophysical Journal</i> , 2016, 832, 213.	1.6	9
7701	<i>Ab initio</i> modeling of steady-state and time-dependent charge transport in hole-only μ -NPD devices. <i>Applied Physics Letters</i> , 2016, 109, .	1.5	12
7702	Microscopic origin of the charge transfer in single crystals based on thiophene derivatives: A combined NEXAFS and density functional theory approach. <i>Journal of Chemical Physics</i> , 2016, 145, 034702.	1.2	12

#	ARTICLE	IF	CITATIONS
7703	Self-consistent implementation of ensemble density functional theory method for multiple strongly correlated electron pairs. <i>Journal of Chemical Physics</i> , 2016, 145, 244104.	1.2	23
7704	Reactions of the Lithiated Diphosphine $(i\text{-}t\text{-}i)\text{Bu}_2\text{P}(\text{SiMe}_3)\text{Li}$ with $[(\text{i-}t\text{-}i)\text{C}_6\text{H}_6]\text{RuCl}_2$ in the Presence of Tertiary Phosphines. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 4241-4249.	1.0	4
7705	A Database of the Structural and Electronic Properties of Prussian Blue, Prussian White, and Berlin Green Compounds through Density Functional Theory. <i>Inorganic Chemistry</i> , 2016, 55, 12851-12862.	1.9	92
7706	Quantum Monte Carlo Calculations on the Anomeric Effect. <i>ACS Symposium Series</i> , 2016, , 89-105.	0.5	1
7707	Quantum tunneling during interstellar surface-catalyzed formation of water: the reaction $\text{H}_2\text{O} + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O} + \text{OH}$. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 33021-33030.	1.3	36
7708	Tight-binding approximations to time-dependent density functional theory – A fast approach for the calculation of electronically excited states. <i>Journal of Chemical Physics</i> , 2016, 144, 184103.	1.2	40
7709	Theoretical study of the decomposition pathways and products of C5- perfluorinated ketone (C5 PFK). <i>AIP Advances</i> , 2016, 6, .	0.6	50
7710	The Symmetric Exchange Reaction $\text{OH} + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O} + \text{OH}$: Convergent Quantum Mechanical Predictions. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10223-10230.	1.1	23
7711	Charge transport properties of graphene: Effects of Cu-based gate electrode. <i>Journal of Applied Physics</i> , 2016, 120, .	1.1	1
7712	Understanding the difference in cohesive energies between alpha and beta tin in DFT calculations. <i>AIP Advances</i> , 2016, 6, .	0.6	27
7713	Mechanisms for the deamination reaction of 8-oxoguanine catalyzed by 8-oxoguanine deaminase: A combined QM/MM molecular dynamics study. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650066.	1.8	1
7714	Improving the accuracy of ground-state correlation energies within a plane-wave basis set: The electron-hole exchange kernel. <i>Journal of Chemical Physics</i> , 2016, 145, 104105.	1.2	18
7715	Excess electrons in methanol clusters: Beyond the one-electron picture. <i>Journal of Chemical Physics</i> , 2016, 145, 164313.	1.2	5
7716	A polarizable QM/MM approach to the molecular dynamics of amide groups solvated in water. <i>Journal of Chemical Physics</i> , 2016, 144, 114504.	1.2	14
7717	Ultra-fast computation of electronic spectra for large systems by tight-binding based simplified Tamm-Dancoff approximation (sTDA-xTB). <i>Journal of Chemical Physics</i> , 2016, 145, 054103.	1.2	115
7718	Perspective: Kohn-Sham density functional theory descending a staircase. <i>Journal of Chemical Physics</i> , 2016, 145, 130901.	1.2	243
7719	UV excitations of halons. <i>Journal of Chemical Physics</i> , 2016, 145, 184306.	1.2	6
7720	Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections. <i>Journal of Chemical Physics</i> , 2016, 145, 204101.	1.2	26

#	ARTICLE	IF	CITATIONS
7721	The impact of electron correlations on the energetics and stability of silicon nanoclusters. <i>Journal of Chemical Physics</i> , 2016, 145, 074313.	1.2	7
7722	Photodynamics of oxybenzone sunscreen: Nonadiabatic dynamics simulations. <i>Journal of Chemical Physics</i> , 2016, 145, 074308.	1.2	41
7723	Terminal Modulation of D π - π^* A Small Molecule for Organic Photovoltaic Materials: A Theoretical Molecular Design. <i>Journal of Physical Chemistry C</i> , 2016, 120, 28939-28950.	1.5	41
7724	Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. <i>Journal of Chemical Physics</i> , 2016, 144, 074106.	1.2	117
7725	Effect of Out-of-Plane Alkyl Group's Position in Dye-Sensitized Solar Cell Efficiency: A Structure-Property Relationship Utilizing Indoline-Based Unsymmetrical Squaraine Dyes. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 35353-35367.	4.0	63
7727	Hybrid density functional study on lattice vibration, thermodynamic properties, and chemical bonding of plutonium monocarbide. <i>Chinese Physics B</i> , 2016, 25, 067106.	0.7	1
7728	Investigating the electronic structure of a supported metal nanoparticle: Pd in SiCN. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31966-31972.	1.3	4
7729	Multi-state extrapolation of UV/Vis absorption spectra with QM/QM hybrid methods. <i>Journal of Chemical Physics</i> , 2016, 144, 184102.	1.2	5
7730	In-situ TEM observation of rock salt crystal precipitation in liposome. <i>MRS Advances</i> , 2016, 1, 1871-1876.	0.5	0
7731	Time-dependent density functional theory (TD-DFT) coupled with reference interaction site model self-consistent field explicitly including spatial electron density distribution (RISM-SCF-SEDD). <i>Journal of Chemical Physics</i> , 2016, 145, 094101.	1.2	19
7732	The mechanism of hydrogen abstraction by high valence transition metal oxo compounds. <i>Journal of Energy Chemistry</i> , 2016, 25, 1045-1050.	7.1	2
7733	Insights into the Phosphoryl Transfer Mechanism of Human Ubiquitous Mitochondrial Creatine Kinase. <i>Scientific Reports</i> , 2016, 6, 38088.	1.6	7
7734	Comparing two tetraalkylammonium ionic liquids. II. Phase transitions. <i>Journal of Chemical Physics</i> , 2016, 144, 224505.	1.2	27
7735	Enhanced ordering reduces electric susceptibility of liquids confined to graphene slit pores. <i>Scientific Reports</i> , 2016, 6, 27406.	1.6	13
7736	Accelerating molecular property calculations with nonorthonormal Krylov space methods. <i>Journal of Chemical Physics</i> , 2016, 144, 174105.	1.2	50
7737	Bond energies of ThO ⁺ and ThC ⁺ : A guided ion beam and quantum chemical investigation of the reactions of thorium cation with O ₂ and CO. <i>Journal of Chemical Physics</i> , 2016, 144, 184309.	1.2	48
7738	Theoretical Investigation of Regioselectivity and Stereoselectivity in AIBN/H ₃ SnBu ₃ -Mediated Radical Cyclization of <i>N</i> -(2-Iodo-4,6-dimethylphenyl)- <i>N</i> ,2-dimethyl-(2- <i>E</i>)-butenamide. <i>Journal of Physical Chemistry B</i> , 2016, 120, 12950-12958.	1.2	6
7739	On the applicability of one- and many-electron quantum chemistry models for hydrated electron clusters. <i>Journal of Chemical Physics</i> , 2016, 144, 154311.	1.2	17

#	ARTICLE	IF	CITATIONS
7740	Electronic spectrum of 9-methylantracene radical cation. <i>Journal of Chemical Physics</i> , 2016, 144, 154303.	1.2	0
7741	Gas phase structures and charge localization in small aluminum oxide anions: Infrared photodissociation spectroscopy and electronic structure calculations. <i>Journal of Chemical Physics</i> , 2016, 144, 244305.	1.2	13
7742	Optimized virtual orbital subspace for faster GW calculations in localized basis. <i>Journal of Chemical Physics</i> , 2016, 145, 234110.	1.2	24
7743	Different conical intersections control nonadiabatic photochemistry of fluorene light-driven molecular rotary motor: A CASSCF and spin-flip DFT study. <i>Journal of Chemical Physics</i> , 2016, 145, 244311.	1.2	21
7744	Design a better metalloporphyrin semiconductor: A theoretical studies on the effect of substituents and central ions. <i>AIP Conference Proceedings</i> , 2016, .	0.3	8
7745	Exciton Splitting of Adsorbed and Free 4-Nitroazobenzene Dimers: A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3055-3070.	1.1	16
7746	Radiation damage in X-ray crystallography: a quantum-mechanical study of photoinduced defect formation in beeswax-analogue n-icosane crystals. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	3
7747	Role of (H ₂ O) _n (n = 2-3) Clusters on the HO ₂ + O ₃ Reaction: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1560-1568.	1.2	26
7748	A Systematic Study on the Influence of Electron-Acceptors in Phenanthrocarbazole Dye-Sensitized Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 9839-9848.	4.0	32
7749	Metal-interacted histidine dimer: an ETS-NOCV and XANES study. <i>RSC Advances</i> , 2016, 6, 38919-38930.	1.7	5
7750	Quantum Mechanical and Absorption Spectral Characterization of Rhodamine B in Ternary Solution. <i>Analytical Letters</i> , 2016, 49, 2606-2614.	1.0	3
7751	A dataset of highly accurate homolytic Ni-Br bond dissociation energies obtained by Means of W2 theory. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 52-60.	1.0	28
7752	Semiconducting and optical properties of selected binary compounds by linear response DFT+U and hybrid functional methods. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	13
7753	Hybrid Density Functionals Applied to Complex Solid Catalysts: Successes, Limitations, and Prospects. <i>Catalysis Letters</i> , 2016, 146, 861-885.	1.4	31
7754	Theoretical investigation on activation of CH and CC bonds of 2-butyne by gas-phase Nb atom. <i>Computational and Theoretical Chemistry</i> , 2016, 1085, 23-30.	1.1	7
7755	Exploring the inhibitory potential of bioactive compound from <i>Luffa acutangula</i> against NF- κ B: A molecular docking and dynamics approach. <i>Computational Biology and Chemistry</i> , 2016, 62, 29-35.	1.1	26
7756	Theoretical study on effect of thiophene substitution on the structure and phosphorescence quantum yields of red-emitting iridium(III) emitters in OLEDs. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 319-320, 25-33.	2.0	2
7757	Electronic structure of polythieno[3,4-b]-thiophene-co-benzodithiophene (PTB7) derivatives for organic solar cell applications. <i>Organic Electronics</i> , 2016, 33, 246-252.	1.4	19

#	ARTICLE	IF	CITATIONS
7758	Rhodocomatulin-Type Anthraquinones from the Australian Marine Invertebrates <i>Clathria hirsuta</i> and <i>Comatula rotularia</i> . <i>Journal of Natural Products</i> , 2016, 79, 946-953.	1.5	16
7759	A Series of Novel Derivatives with Giant Second Hyperpolarizabilities, Based on Radiannulenes, Tetrathiafulvalene, Nickel Dithiolene, and Their Lithiated Analogues. <i>Journal of Physical Chemistry C</i> , 2016, 120, 9419-9435.	1.5	25
7760	Excited-State Absorption from Real-Time Time-Dependent Density Functional Theory: Optical Limiting in Zinc Phthalocyanine. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1387-1391.	2.1	31
7761	Reaction pathway of coal oxidation at low temperatures: a model of cyclic chain reactions and kinetic characteristics. <i>Combustion and Flame</i> , 2016, 163, 447-460.	2.8	244
7762	Selective Co-Oligomerization of Ethylene and 1-Hexene by Chromium-PNP Catalysts: A DFT Study. <i>Organometallics</i> , 2016, 35, 972-981.	1.1	29
7763	Methionine one-electron oxidation: Coherent contributions from radiolysis, IRMPD spectroscopy, DFT calculations and electrochemistry. <i>Radiation Physics and Chemistry</i> , 2016, 128, 103-111.	1.4	15
7764	Mechanism of the Reaction of Human Manganese Superoxide Dismutase with Peroxynitrite: Nitration of Critical Tyrosine 34. <i>Biochemistry</i> , 2016, 55, 3403-3417.	1.2	37
7765	Reaction of a 2,4,6-triphenylphosphinine ferrate anion with electrophiles: a new route to phosphacyclohexadienyl complexes. <i>Dalton Transactions</i> , 2016, 45, 8875-8884.	1.6	9
7766	Electronic and Optical Properties of the Narrowest Armchair Graphene Nanoribbons Studied by Density Functional Methods. <i>Australian Journal of Chemistry</i> , 2016, 69, 960.	0.5	10
7767	Stiff-stilbene photoswitch ruptures bonds not by pulling but by local heating. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15848-15853.	1.3	12
7768	Density Functional Theory. <i>Graduate Texts in Physics</i> , 2016, , 99-110.	0.1	1
7769	DFT study of zigzag (n, 0) single-walled carbon nanotubes: ¹³ C NMR chemical shifts. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 67, 14-19.	1.3	16
7770	New manganese(II) and nickel(II) coordination compounds with N,O-polydentate ligands obtained from pyridoxal and tripodal units. <i>Journal of Molecular Structure</i> , 2016, 1120, 163-170.	1.8	6
7771	Quantum chemical investigation on the structural and electronic properties of $\hat{1}^{\pm}$ -, $\hat{1}^{2-}$ -, and $\hat{1}^{3-}$ -cyclodextrin complexes: DFT and QTAIM analysis. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 1192-1199.	0.1	7
7772	A DFT study on adsorption behaviour of CO on Co ₃ O ₄ nanostructures. <i>Applied Surface Science</i> , 2016, 385, 113-121.	3.1	26
7773	Cations or Radicals? Inherent Reactivity of Biosynthetic Intermediates in the B-Ring Formation of Rotenoid Natural Products. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2372-2379.	1.1	1
7774	Packing of Large Two- and Three-Photon Activity Into Smallest Possible Unsymmetrical Fluorene Chromophores. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2757-2770.	1.1	7
7775	Oxidative Addition of the N-H Bond of Ammonia to Iridium Bis(phosphane) Complexes: A Combined Experimental and Theoretical Study. <i>Organometallics</i> , 2016, 35, 720-731.	1.1	16

#	ARTICLE	IF	CITATIONS
7776	Ab initio study of the enantio-selective magnetic-field-induced second harmonic generation in chiral molecules. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1846-1858.	1.3	3
7777	Electronic communication in phosphine substituted bridged dirhenium complexes – clarifying ambiguities raised by the redox non-innocence of the C ₄ H ₂ - and C ₄ -bridges. <i>Dalton Transactions</i> , 2016, 45, 5783-5799.	1.6	18
7778	Captodative substitution induced acceleration effect towards 4π electrocyclic ring-opening of substituted cyclobutenes. <i>RSC Advances</i> , 2016, 6, 25503-25510.	1.7	6
7779	Density functional theory study of the mechanism of a dipeptide-catalyzed intermolecular aldol reaction – the effects of steric repulsion interactions on stereoselectivity. <i>RSC Advances</i> , 2016, 6, 19742-19750.	1.7	2
7780	DFT modeling of adsorption of formaldehyde and methanediol anion on the (111) face of IB metals. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 122-129.	0.1	3
7781	Optical absorption spectrum of the N3 solar cell sensitizer by second-order multireference perturbation theory. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	11
7782	Photoleucine Survives Backbone Cleavage by Electron Transfer Dissociation. A Near-UV Photodissociation and Infrared Multiphoton Dissociation Action Spectroscopy Study. <i>Journal of the American Society for Mass Spectrometry</i> , 2016, 27, 1176-1185.	1.2	11
7783	Prediction of neutral noble gas insertion compounds with heavier pnictides: FN ₃ Y (Ng = Kr and Xe; Y =) Tj ETQq1 1 0,784314,rgBT /Over	1.3	21
7784	On the different strength of photoacids. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	25
7785	The acidity of ¹² P-phosphoglucomutase monofluoromethylenephosphonate ligands probed by NMR spectroscopy and quantum mechanical methods. <i>Canadian Journal of Chemistry</i> , 2016, 94, 902-908.	0.6	2
7786	Intramolecular photo-induced electron transfer in nonlinear optical chromophores: Fullerene (C ₆₀) derivatives. <i>Organic Electronics</i> , 2016, 33, 290-299.	1.4	27
7787	Ligand-Binding Affinity Estimates Supported by Quantum-Mechanical Methods. <i>Chemical Reviews</i> , 2016, 116, 5520-5566.	23.0	216
7788	Using density functional theory to calculate the anomeric effect in hydroxylamine and hydrazide derivatives of tetrahydropyran. <i>Journal of Carbohydrate Chemistry</i> , 2016, 35, 106-117.	0.4	0
7789	A PW91-like exchange with a simple analytical form. <i>Chemical Physics Letters</i> , 2016, 651, 268-273.	1.2	16
7790	Kinetics of CO ₂ capture by carbon dioxide binding organic liquids: Experimental and molecular modelling studies. <i>International Journal of Greenhouse Gas Control</i> , 2016, 49, 379-386.	2.3	18
7791	Light induced intramolecular electron and energy transfer events in rigidly linked borondipyromethene: Corrole Dyad. <i>Journal of Luminescence</i> , 2016, 177, 209-218.	1.5	19
7792	Choosing an appropriate model chemistry in a big data context: Application to dative bonding. <i>Computational and Theoretical Chemistry</i> , 2016, 1085, 46-55.	1.1	2
7793	Dispersion-Corrected Mean-Field Electronic Structure Methods. <i>Chemical Reviews</i> , 2016, 116, 5105-5154.	23.0	1,032

#	ARTICLE	IF	CITATIONS
7794	Theoretical Insights into the Mechanism of CO ₂ Chemisorption and Subsequent CO Desorption on Char Surface with Zigzag Active Sites. <i>Combustion Science and Technology</i> , 2016, 188, 1136-1151.	1.2	4
7795	Expensive tripod rotation in η^6 -chromium tricarbonyl complexes of phosphabenzene-Insights from DFT study. <i>Computational and Theoretical Chemistry</i> , 2016, 1084, 103-108.	1.1	2
7796	Exploring the role of a single water molecule in the tropospheric reaction of glycolaldehyde with an OH radical: a mechanistic and kinetics study. <i>RSC Advances</i> , 2016, 6, 29080-29098.	1.7	15
7797	Study on the removal of benzisothiazolinone biocide and its toxicity: The effectiveness of ozonation. <i>Chemical Engineering Journal</i> , 2016, 300, 376-383.	6.6	44
7798	Parquet compounds on the basis of eight- and twelve-membered structure blocks: Quantum-chemical study. <i>Russian Journal of Organic Chemistry</i> , 2016, 52, 268-282.	0.3	3
7799	Global hybrid exchange energy functional with correct asymptotic behavior of the corresponding potential. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	7
7800	Apoptotic effect of eugenol involves G2/M phase abrogation accompanied by mitochondrial damage and clastogenic effect on cancer cell in vitro. <i>Phytomedicine</i> , 2016, 23, 725-735.	2.3	43
7801	A broken-symmetry density functional study of structures, energies, and protonation states along the catalytic O-H bond cleavage pathway in ba3 cytochrome c oxidase from <i>Thermus thermophilus</i> . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21162-21171.	1.3	21
7802	An amide functionalized task specific carbon nanotube for the sorption of tetra and hexa valent actinides: experimental and theoretical insight. <i>RSC Advances</i> , 2016, 6, 39553-39562.	1.7	54
7803	Carnosine and Homocarnosine Degradation Mechanisms by the Human Carnosinase Enzyme CN1: Insights from Multiscale Simulations. <i>Biochemistry</i> , 2016, 55, 2772-2784.	1.2	20
7804	A new oxorhenium(V) complex with benzothiazole derived ligand: Relative stability and global chemical reactivity indices. <i>Inorganica Chimica Acta</i> , 2016, 447, 168-175.	1.2	20
7805	Magnetic properties with multiwavelets and DFT: the complete basis set limit achieved. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21145-21161.	1.3	40
7806	The fragment molecular orbital method combined with density-functional tight-binding and the polarizable continuum model. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22047-22061.	1.3	59
7807	The ultrafast reactions in the photochromic cycle of water-soluble fulgimide photoswitches. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10289-10296.	1.3	18
7808	A density functional theory investigation of the reactions of Fe and FeO ₂ with O ₂ . <i>Computational Materials Science</i> , 2016, 117, 455-467.	1.4	8
7809	Synthesis, structure, DFT calculations, electrochemistry, fluorescence, DNA binding and molecular docking aspects of a novel oxime based ligand and its palladium(II) complex. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2016, 160, 336-346.	1.7	28
7810	Completing the Heterocubane Family [Cp*AlE] ₄ (E = O, S, Se, and Te) by Selective Oxygenation and Sulfuration of [Cp*Al] ₄ : Density Functional Theory Calculations of [Cp*AlE] ₄ and Reactivity of [Cp*AlO] ₄ toward Hydrolysis. <i>Inorganic Chemistry</i> , 2016, 55, 4915-4923.	1.9	38
7811	Evaluating the <i>i</i> -GW Approximation with CCSD(T) for Charged Excitations Across the Oligoacenes. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2834-2842.	2.3	71

#	ARTICLE	IF	CITATIONS
7812	Exploring the origin of the anomeric relationships in 2-cyanooxane, 2-cyanothiane, 2-cyanoselenane and their corresponding isocyano isomers. Correlations between hyper-conjugative anomeric effect, hardness and electrostatic interactions. <i>RSC Advances</i> , 2016, 6, 46406-46420.	1.7	10
7813	Femtosecond structural dynamics drives the trans/cis isomerization in photoactive yellow protein. <i>Science</i> , 2016, 352, 725-729.	6.0	348
7814	A series of diphenylamine-fluorenone derivatives as potential fluorescent probes for neuroblastoma cell staining. <i>Tetrahedron</i> , 2016, 72, 2920-2928.	1.0	17
7815	Fe(100)â€“(borazine) _{n=1-4} â€“(Fe(100): a multifunctional spin diode with spin valve action. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14376-14381.	1.3	8
7816	Structures and Binding Energies of the Naphthalene Dimer in Its Ground and Excited States. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2779-2782.	1.1	28
7817	Connecting effect on the first hyperpolarizability of armchair carbonâ€“(boronâ€“(nitride heteronanotubes: pattern versus proportion. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 13954-13959.	1.3	17
7818	Assessing the formation of weak sodium complexes with negatively charged ligands. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 13118-13125.	1.3	4
7819	Spectroscopic, electrochemical, theoretical characterization and biological evaluation of a ferrocenyl-substituted unsymmetric azine ligand and its Cu(II) complex. <i>Journal of Coordination Chemistry</i> , 2016, 69, 1587-1601.	0.8	6
7820	Structural and spectroscopic characterization of epiisopiloturine-metal complexes, and anthelmintic activity <i>vs</i> <i>S. mansoni</i> . <i>Journal of Coordination Chemistry</i> , 2016, 69, 1663-1683.	0.8	5
7821	Synthesis and Comprehensive Structural and Chiroptical Characterization of Enones Derived from (â€“(â€“(Santonin by Experiment and Theory. <i>Journal of Organic Chemistry</i> , 2016, 81, 4588-4600.	1.7	13
7822	Unfolding ESIPT in Bis-2,5-(2-benzoxazolyl) Hydroquinone and 2,5-Bis(benzo[d]oxazol-2-yl)-4-methoxyphenol: a Comprehensive Computational Approach. <i>Journal of Fluorescence</i> , 2016, 26, 1295-1307.	1.3	4
7823	Uncatalyzed thermal gas phase aziridination of alkenes by organic azides. Part I: Mechanisms with discrete nitrene species. <i>Journal of Chemical Sciences</i> , 2016, 128, 681-693.	0.7	4
7824	A Projector-Embedding Approach for Multiscale Coupled-Cluster Calculations Applied to Citrate Synthase. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2689-2697.	2.3	58
7825	Rare-earth pnictides and chalcogenides from first-principles. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 223001.	0.7	24
7826	Computational Exploration of Rh ^{III} /Rh ^V and Rh ^{III} /Rh ^I Catalysis in Rhodium(III)-Catalyzed Câ€“(H Activation Reactions of <i>N</i> -Phenoxyacetamides with Alkynes. <i>Journal of the American Chemical Society</i> , 2016, 138, 6861-6868.	6.6	116
7827	Computational kinetic modeling of the selenol catalytic activity as the glutathione peroxidase nanomimic. <i>Journal of Theoretical Biology</i> , 2016, 409, 108-114.	0.8	5
7828	An efficient DFT method of predicting the one-, two- and three-bond indirect spinâ€“(spin coupling constants involving a fluorine nucleus in fluoroalkanes. <i>RSC Advances</i> , 2016, 6, 82783-82792.	1.7	14
7829	Free energy barrier for dissociation of the guanosine monophosphate anion in water. <i>European Physical Journal D</i> , 2016, 70, 1.	0.6	11

#	ARTICLE	IF	CITATIONS
7830	Density Functional Theory Methods for Computing and Predicting Mechanical Properties. Springer Series in Materials Science, 2016, , 131-158.	0.4	0
7831	Novel Rhodafluors: Synthesis, Photophysical, pH and TD-DFT Studies. Journal of Fluorescence, 2016, 26, 2187-2197.	1.3	9
7832	The Importance of Methyl Positioning and Tautomeric Equilibria for Imidazole Nucleophilicity. Chemistry - A European Journal, 2016, 22, 15521-15528.	1.7	11
7833	Self-Consistent Constricted Variational Theory RSCF-CV($\hat{\alpha}^{\hat{z}}$)-DFT and Its Restrictions To Obtain a Numerically Stable \hat{T}^{SCF} -DFT-like Method: Theory and Calculations for Triplet States. Journal of Chemical Theory and Computation, 2016, 12, 5438-5452.	2.3	12
7834	Catalysts for Isocyanate-Free Polyurea Synthesis: Mechanism and Application. ACS Catalysis, 2016, 6, 6883-6891.	5.5	48
7835	Rapid Hydrogen and Oxygen Atom Transfer by a High-Valent Nickel O^{O} Oxygen Species. Journal of the American Chemical Society, 2016, 138, 12987-12996.	6.6	66
7836	Exploring the Intricacies of Weak Interactions in Metal O^{M} Metal Bonds Using an Unsymmetrical Carbonyl Precursor and a Triple-Bonded W ₂ ⁶⁺ Paddlewheel. Inorganic Chemistry, 2016, 55, 9471-9481.	1.9	3
7837	Implementation of Molecular Gradients for Local Hybrid Density Functionals Using Seminumerical Integration Techniques. Journal of Chemical Theory and Computation, 2016, 12, 4254-4262.	2.3	33
7838	Interaction-Strength Interpolation Method for Main-Group Chemistry: Benchmarking, Limitations, and Perspectives. Journal of Chemical Theory and Computation, 2016, 12, 4885-4896.	2.3	34
7839	X-Ray absorption spectra of microsolvated metal cations. Physical Chemistry Chemical Physics, 2016, 18, 16671-16681.	1.3	5
7840	Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. Chemical Communications, 2016, 52, 13840-13860.	2.2	18
7841	Unimolecular dissociation of peptides: statistical vs. non-statistical fragmentation mechanisms and time scales. Faraday Discussions, 2016, 195, 599-618.	1.6	27
7842	Electronic structure and magnetism of samarium and neodymium adatoms on free-standing graphene. Physical Review B, 2016, 94, .	1.1	22
7843	Weakly bounded intermediates as a previous step towards highly-enantioselective iminium type additions of I^2 -keto-sulfoxides and -sulfones. Journal of Molecular Catalysis A, 2016, 423, 308-318.	4.8	9
7844	Structure and electronics properties of novel antimalarial molecules: Comparative study of ferrotriborodiaziquine and ferrodiborotriazoquinone with ferroquinone using density functional theory. Polyhedron, 2016, 119, 471-482.	1.0	1
7845	Mechanistic Investigation of Molybdate O^{M} Catalysed Transfer Hydrodeoxygenation. Chemistry - A European Journal, 2016, 22, 16621-16631.	1.7	20
7846	2D Structures Beyond Graphene. Semiconductors and Semimetals, 2016, 95, 1-33.	0.4	8
7847	Investigation of the identity of the nucleophile initiating the hydrolysis of phosphate esters catalyzed by dinuclear mimics of metallohydrolases. Journal of Inorganic Biochemistry, 2016, 162, 356-365.	1.5	7

#	ARTICLE	IF	CITATIONS
7848	Benchmarking Electron Densities and Electrostatic Potentials of Proteins from the Three-Partition Frozen Density Embedding Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4843-4855.	2.3	11
7849	Thermal Decomposition Kinetics of Dicyclopentadiene-1,8-dione: The Reaction Path through Quantum Chemical Calculation. <i>International Journal of Chemical Kinetics</i> , 2016, 48, 812-821.	1.0	1
7850	Calculations of the light absorption spectra of porphyrinoid chromophores for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27877-27884.	1.3	8
7851	Probing the potential of halogen-free superhalogen anions as effective electrolytes of Li-ion batteries: a theoretical prospect from combined ab initio and DFT studies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28576-28584.	1.3	25
7852	Highly stereoselective metal-mediated domino aldol reactions of propiophenone enolates with heteroaromatic, aliphatic, and unsaturated aldehydes. <i>Monatshefte für Chemie</i> , 2016, 147, 1925-1932.	0.9	0
7853	Benchmarking the DFT methodology for assessing antioxidant-related properties: quercetin and edaravone as case studies. <i>Journal of Molecular Modeling</i> , 2016, 22, 250.	0.8	24
7854	meta-Benzoporphodimethenes: New Cell Imaging Porphyrin Analogue Molecules. <i>ChemistrySelect</i> , 2016, 1, 3502-3509.	0.7	6
7855	First-Principles Study of Nonradiative Recombination in Silicon Nanocrystals: The Role of Surface Silanol. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23246-23253.	1.5	12
7856	Spin-state energies of heme-related models from spin-flip TDDFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29486-29494.	1.3	9
7857	Electrocatalytic reduction of carbon dioxide with Mn(terpyridine) carbonyl complexes. <i>Dalton Transactions</i> , 2016, 45, 17179-17186.	1.6	40
7858	Computational electrochemistry study of derivatives of anthraquinone and phenanthraquinone analogues: the substitution effect. <i>RSC Advances</i> , 2016, 6, 89827-89835.	1.7	18
7859	Temperature Dual Enantioselective Control in a Rhodium-Catalyzed Michael-Type Friedel-Crafts Reaction: A Mechanistic Explanation. <i>Chemistry - A European Journal</i> , 2016, 22, 11064-11083.	1.7	22
7860	C-N Bond Coupling Reactions of Ammonia with Acetone Promoted by Iridium and Rhodium Complexes: Experimental and DFT Studies. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5347-5355.	1.0	2
7861	The role of dispersive forces determining the energetics of adsorption in Ti zeolites. <i>Journal of Computational Chemistry</i> , 2016, 37, 2659-2666.	1.5	8
7862	Study of the thermal conversions of organic carbon of Huadian oil shale during pyrolysis. <i>Energy Conversion and Management</i> , 2016, 127, 284-292.	4.4	39
7863	Redox Behavior of the S-Adenosylmethionine (SAM)-Binding Fe-S Cluster in Methylthiotransferase RimO, toward Understanding Dual SAM Activity. <i>Biochemistry</i> , 2016, 55, 5798-5808.	1.2	13
7864	Solvent effects on the properties of hyperbranched polythiophenes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24610-24619.	1.3	0
7865	Quantum chemical study of the (Z)-2-penten-1-ol (HOCH ₂ CH=CHCH ₂ CH ₃) + OH + O ₂ reactions. <i>Molecular Physics</i> , 2016, 114, 3183-3192.	0.8	1

#	ARTICLE	IF	CITATIONS
7866	Surface properties of hydrogenated diamond in the presence of adsorbates: A hybrid functional DFT study. <i>Carbon</i> , 2016, 110, 469-479.	5.4	38
7867	Imaging the Nonlinear Susceptibility Tensor of Collagen by Nonlinear Optical Stokes Ellipsometry. <i>Biophysical Journal</i> , 2016, 111, 1361-1374.	0.2	26
7868	Influence of Ring-Expanded <i>N</i> -Heterocyclic Carbenes on the Structures of Half-Sandwich Ni(I) Complexes: An X-ray, Electron Paramagnetic Resonance (EPR), and Electron Nuclear Double Resonance (ENDOR) Study. <i>Inorganic Chemistry</i> , 2016, 55, 11006-11017.	1.9	25
7869	A comparison of the experimental and theoretical charge density distributions in two polymorphic modifications of piroxicam. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28802-28818.	1.3	15
7870	Structural transformations in the carborane series: C ₂ B ₆ H ₆ (n= 0-6) upon substitution of boron by carbon. <i>Inorganica Chimica Acta</i> , 2016, 453, 626-632.	1.2	7
7871	An analysis of the experimental and theoretical charge density distributions of the piroxicam-saccharin co-crystal and its constituents. <i>RSC Advances</i> , 2016, 6, 81578-81590.	1.7	18
7872	Application of the dielectric-dependent screened exchange potential approach to organic photocell materials. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27554-27563.	1.3	18
7873	Radical-induced dissociation leading to the loss of CO ₂ from the oxazolone ring of [b ⁵ H]E TM +ions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18119-18127.	1.3	2
7874	Experimental and Theoretical Study of the High-Temperature UV-Visible Spectra of Aqueous Hydroquinone and 1,4-Benzoquinone. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10547-10552.	1.2	4
7875	Structure, Ionization, and Fragmentation of Hydrogenated Aluminoboron Clusters: Al ₂ B ₂ H _{2n} (n=0-6). <i>ChemistrySelect</i> , 2016, 1, 3804-3811.	0.7	3
7876	The effect of heterocyclic π bridges on second order nonlinear optical properties of compounds formed between ferrocenyl and corannulene. <i>RSC Advances</i> , 2016, 6, 97063-97069.	1.7	9
7877	Stereoisomers of an azine-linked donor-acceptor conjugated polymer: the impact of molecular conformation on electrical performance. <i>RSC Advances</i> , 2016, 6, 44272-44278.	1.7	8
7878	B88 exchange functional recovering the local spin density linear response. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	2
7879	Selectivity of peptide bond dissociation on excitation of a core electron: Effects of a phenyl group. <i>Chemical Physics Letters</i> , 2016, 660, 60-68.	1.2	7
7880	Insight into the Excited State Electronic and Structural Properties of the Organic Photovoltaic Donor Polymer Poly(thieno[3,4- <i>b</i>]thiophene benzodithiophene) by Means of <i>ab Initio</i> and Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21818-21826.	1.5	22
7881	The synthesis of a pyridine-N-oxide isophthalamide rotaxane utilizing supplementary amide hydrogen bond interactions. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 7972-7981.	1.5	10
7882	The 1,2-hydrogen shift reaction for monohalogenophosphanes PH ₂ X and HPX (X= F, Cl). <i>Molecular Physics</i> , 2016, 114, 2999-3014.	0.8	3
7883	General approach for band gap calculation of semiconductors and insulators. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2016, 213, 2834-2837.	0.8	8

#	ARTICLE	IF	CITATIONS
7884	Polymerization of Thienothiophenes and Dithienothiophenes via Click-Reaction for Electronic Applications. <i>ChemistrySelect</i> , 2016, 1, 3028-3032.	0.7	11
7885	Effects of the acceptor unit in dyes with acceptor-bridge-donor architecture on the electron photo-injection mechanism and aggregation in DSSCs. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24239-24251.	1.3	23
7886	The highly enantioselective bifunctional organocatalysts for the Michael addition of γ -cyclohexanone to nitroolefins. <i>Russian Journal of General Chemistry</i> , 2016, 86, 1381-1388.	0.3	1
7887	DFT 101 and Applications to π -Conjugated Systems. <i>Materials and Energy</i> , 2016, , 19-52.	2.5	0
7888	Ab Initio Benchmark Study of Nonadiabatic S1-S2 Photodynamics of cis- and trans-Hexatriene. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6541-6556.	1.1	10
7889	Mechanistically Inspired Route toward Hexahydro-2H-chromenes via Consecutive [4 + 2] Cycloadditions. <i>Organic Letters</i> , 2016, 18, 3976-3979.	2.4	11
7890	Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists. <i>Accounts of Chemical Research</i> , 2016, 49, 1503-1513.	7.6	103
7891	Topological Study of Bonding in Aquo and Bis(triazinyl)pyridine Complexes of Trivalent Lanthanides and Actinides: Does Covalency Imply Stability?. <i>Inorganic Chemistry</i> , 2016, 55, 10034-10042.	1.9	41
7892	Half-sandwich complexes of rhodium containing cysteine-derived ligands. <i>Dalton Transactions</i> , 2016, 45, 14203-14215.	1.6	3
7893	A D-A-A metal-free organic dye with improved efficiency for the application of solar energy conversion. <i>Dyes and Pigments</i> , 2016, 134, 498-505.	2.0	29
7894	Effect of End Groups on Mechanochromism and Electroluminescence in Tetraphenylethylene Substituted Phenanthroimidazoles. <i>Journal of Physical Chemistry C</i> , 2016, 120, 18487-18495.	1.5	82
7895	Aggregation of metal-free organic sensitizers on TiO ₂ (1 0 1) surface for use in dye-sensitized solar cells: A computational investigation. <i>Computational and Theoretical Chemistry</i> , 2016, 1093, 1-8.	1.1	10
7896	Synthesis and photovoltaic performance of dibenzofulvene-based organic sensitizers for DSSC. <i>Tetrahedron</i> , 2016, 72, 5788-5797.	1.0	5
7897	Mechanistic Photochemistry of Methyl-4-hydroxycinnamate Chromophore and Its One-Water Complexes: Insights from MS-CASPT2 Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6014-6022.	1.1	23
7898	Reaction of Phenyl Iso(thio)cyanate with N-Heterocyclic Carbene-Supported Nickel Complexes: Formation of Nickelacycles. <i>Organometallics</i> , 2016, 35, 2722-2727.	1.1	21
7899	Addition and abstraction reaction mechanism of 2,4,5-trimethylphenol with OH radical - A first principle study. <i>Computational and Theoretical Chemistry</i> , 2016, 1092, 90-107.	1.1	10
7900	Origins of the Relative Stabilities of Anhydrous and Hydrated α -Mannitol Crystals. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6629-6636.	1.1	15
7901	Recent application of calculations of metal complexes based on density functional theory. <i>RSC Advances</i> , 2016, 6, 77375-77395.	1.7	47

#	ARTICLE	IF	CITATIONS
7902	Postcombustion CO ₂ Capture Solvent Characterization Employing the Explicit Solvation Shell Model and Continuum Solvation Models. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9034-9050.	1.2	20
7903	The INV24 test set: how well do quantum-chemical methods describe inversion and racemization barriers?. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1133-1143.	0.6	45
7904	Photoreactions with a Twist: Atropisomerism-Driven Divergent Reactivity of Enones with UV and Visible Light. <i>Chemistry - A European Journal</i> , 2016, 22, 11339-11348.	1.7	16
7905	A Modular Class of Fluorescent Difluoroboranes: Synthesis, Structure, Optical Properties, Theoretical Calculations and Applications for Biological Imaging. <i>Chemistry - A European Journal</i> , 2016, 22, 12430-12438.	1.7	32
7906	Changing the chemical and physical properties of high valent heterobimetallic bis-(η^4 -oxido) Cu ^{II} -Ni complexes by ligand effects. <i>Dalton Transactions</i> , 2016, 45, 15994-16000.	1.6	10
7907	Structural features of the carbon-sulfur chemical bond: a semi-experimental perspective. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1065-1076.	0.6	40
7908	A Vanadium Chalcogenide Dicubane. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 28-32.	1.0	4
7909	Investigating the properties of muchimangin B through comparisons with related and model structures. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	0
7910	NLOphoric and solid state emissive BODIPY dyes containing N-phenylcarbazole core at meso position - Synthesis, photophysical properties of and DFT studies. <i>Journal of Luminescence</i> , 2016, 179, 420-428.	1.5	16
7911	Triggering the Chemical Instability of an Ionic Liquid under High Pressure. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9097-9102.	1.2	6
7912	Separation of dynamic and nondynamic correlation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24015-24023.	1.3	85
7913	Promising thermoelectric properties of phosphorenes. <i>Nanotechnology</i> , 2016, 27, 355705.	1.3	43
7914	Toward a Rational Design of Highly Folded Peptide Cation Conformations. 3D Gas-Phase Ion Structures and Ion Mobility Characterization. <i>Journal of the American Society for Mass Spectrometry</i> , 2016, 27, 1647-1660.	1.2	11
7915	A comparative examination of density functional performance against the ISOL24/11 isomerization energy benchmark. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 147-152.	1.1	23
7916	A New Sensitive and Selective Off-On Fluorescent Zn ²⁺ Chemosensor Based on 3,3',5,5'-Tetraphenylsubstituted Dipyromethene. <i>Journal of Fluorescence</i> , 2016, 26, 1967-1974.	1.3	11
7917	Gas phase fragmentation mechanisms of protonated testosterone as revealed by chemical dynamics simulations. <i>International Journal of Mass Spectrometry</i> , 2016, 407, 40-50.	0.7	13
7918	Radical Cations of the Monomer and van der Waals Dimer of a Methionine Residue as Prototypes of (2) Tj ETQq0 0 0 rgBT /Overlock 10 <i>Journal of Physical Chemistry B</i> , 2016, 120, 9875-9886.	1.2	7
7919	Theoretical Assessment of Fluorinated Phospholipids in the Design of Liposomal Drug-Delivery Systems. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9661-9671.	1.2	4

#	ARTICLE	IF	CITATIONS
7920	Density Functional Theory (DFT) and Time Dependent DFT (TDDFT). , 2016, , 155-194.		6
7921	Ab-initio investigation of the finite-temperatures structural, elastic, and thermodynamic properties of Ti ₃ AlC ₂ and Ti ₃ SiC ₂ . Computational Materials Science, 2016, 124, 420-427.	1.4	9
7922	Orbital order switching in molecular calculations using GGA functionals: Qualitative errors in materials modeling for electrochemical power sources and how to fix them. Chemical Physics Letters, 2016, 659, 270-276.	1.2	10
7923	Carbon nanodots as fluorescent platforms for recognition of fluoride ion via the inner filter effect of simple arylboronic acids. Experimental and theoretical investigations. Journal of Fluorine Chemistry, 2016, 190, 12-22.	0.9	15
7924	Multiscale Materials Modeling for Nanomechanics. Springer Series in Materials Science, 2016, , .	0.4	20
7925	Origin of the Absorption Band of Bromophenol Blue in Acidic and Basic pH: Insight from a Combined Molecular Dynamics and TD-DFT/MM Study. Journal of Physical Chemistry A, 2016, 120, 7175-7182.	1.1	5
7926	Theoretical study on photooxidation mechanism of ruthenium complex [Ru(II)â€(bpy) ₂ (TMBiimH ₂) ²⁺ with molecular oxygen. Journal of Computational Chemistry, 2016, 37, 2212-2219.	1.5	5
7927	Copolymers possessing dithienothiophene and boron for optoelectronic applications. Polymer Engineering and Science, 2016, 56, 1390-1398.	1.5	10
7928	Fluoroquinolones: A micro-species equilibrium in the protonation of amphoteric compounds. European Journal of Pharmaceutical Sciences, 2016, 93, 380-391.	1.9	18
7929	Ligand-accelerated enantioselective methylene C(sp ³)â€H bond activation. Science, 2016, 353, 1023-1027.	6.0	296
7930	Excited-state proton transfer in 4-(2-hydroxyphenyl)pyridine: full-dimensional surface-hopping dynamics simulations. RSC Advances, 2016, 6, 85574-85581.	1.7	7
7931	Indole-Based NLOphoric Donor-â€Acceptor Styryl Dyes: Synthesis, Spectral Properties and Computational Studies. Journal of Fluorescence, 2016, 26, 2063-2077.	1.3	11
7932	When Density Functional Approximations Meet Iron Oxides. Journal of Chemical Theory and Computation, 2016, 12, 5132-5144.	2.3	102
7933	Photocycloaddition reaction of atropisomeric maleimides: mechanism and selectivity. Physical Chemistry Chemical Physics, 2016, 18, 24713-24721.	1.3	11
7934	Rhodiumâ€Catalyzed Dehydrogenative Silylation of Acetophenone Derivatives: Formation of Silyl Enol Ethers versus Silyl Ethers. Chemistry - A European Journal, 2016, 22, 14717-14729.	1.7	21
7935	Does Nature Know Best? Pericyclic Reactions in the <i>Daphniphyllum</i> Alkaloid-Forming Cation Cascade. Organic Letters, 2016, 18, 4482-4484.	2.4	16
7936	Iron(III) bis(pyrazol-1-yl)acetate based decanuclear metallacycles: synthesis, structure, magnetic properties and DFT calculations. Dalton Transactions, 2016, 45, 15089-15096.	1.6	10
7937	Rh(III)-Catalyzed Cascade Oxidative Annulation of Benzoylacetone with Alkynes: Computational Study of Mechanism, Reactivity, and Regioselectivity. Journal of Organic Chemistry, 2016, 81, 8378-8385.	1.7	19

#	ARTICLE	IF	CITATIONS
7938	Oxidation state selective sorption behavior of plutonium using N,N-dialkylamide functionalized carbon nanotubes: experimental study and DFT calculation. <i>RSC Advances</i> , 2016, 6, 78692-78701.	1.7	37
7939	Predicted Chemical Activation Rate Constants for HO ₂ + CH ₂ NH: The Dominant Role of a Hydrogen-Bonded Pre-reactive Complex. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7060-7070.	1.1	29
7940	A halogen bond does not dictate the conformational preferences of cis-1,3-disubstituted cyclohexanes. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 8610-8614.	1.5	2
7941	Cryptochirality in 2,2'-Coupled BODIPY DYEimers. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 4236-4243.	1.2	15
7942	Proton-Coupled Electron Transfer in a Strongly Coupled Photosystem II-Inspired Chromophore-Imidazole-Phenol Complex: Stepwise Oxidation and Concerted Reduction. <i>Journal of the American Chemical Society</i> , 2016, 138, 11536-11549.	6.6	66
7943	Adsorption and Dissociation of a Bicyclic Tertiary Diamine, Triethylenediamine, on a Si(100)-2 × 1 Surface. <i>Journal of Physical Chemistry C</i> , 2016, 120, 28672-28681.	1.5	2
7944	Ion-Specific Effects in Carboxylate Binding Sites. <i>Journal of Physical Chemistry B</i> , 2016, 120, 12519-12530.	1.2	41
7945	Computational study of H-abstraction reactions from CH ₃ OCH ₂ CH ₂ Cl/CH ₃ CH ₂ OCH ₂ CH ₂ Cl by Cl atom and OH radical and fate of alkoxy radicals. <i>Environmental Science and Pollution Research</i> , 2016, 23, 23467-23484.	2.7	20
7946	Tetranuclear Lanthanide Complexes Containing a Hydrazone-type Ligand. Dysprosium [2 × 2] Gridlike Single-Molecule Magnet and Toric. <i>Inorganic Chemistry</i> , 2016, 55, 12470-12476.	1.9	43
7947	Understanding the role of hydrogen bonding in Brønsted acidic ionic liquid-catalyzed transesterification: a combined theoretical and experimental investigation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32723-32734.	1.3	14
7948	Anti-tumor activity and mechanism of apoptosis of A549 induced by ruthenium complex. <i>Journal of Biological Inorganic Chemistry</i> , 2016, 21, 945-956.	1.1	14
7949	The synthesis, characterization and computational investigation of a new metalloporphyrine containing 15-membered S ₄ donor macrocyclic moieties. <i>Tetrahedron</i> , 2016, 72, 6972-6981.	1.0	2
7950	Can Strained Hydrocarbons Be "Forced" To Be Stable?. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7198-7204.	1.1	9
7951	Inhibiting the growth of tumor cells by ruthenium(II) complexes [Ru(phen) ₂ L] (L = TFMPIP and p-CPIP) through DNA-binding. <i>Journal of Coordination Chemistry</i> , 2016, 69, 3507-3517.	0.8	3
7952	4-Dimethylaminopyridine-catalyzed dynamic kinetic resolution in asymmetric synthesis of P-chirogenic 1,3,2-oxazaphospholidine-2-oxides. <i>RSC Advances</i> , 2016, 6, 89665-89670.	1.7	7
7953	Theoretical design and characterization of high-efficiency organic dyes with different electron-withdrawing groups based on C275 toward dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2016, 40, 9320-9328.	1.4	18
7954	A Dynamic Equilibrium of Three Hydrogen-Bond Conformers Explains the NMR Spectrum of the Active Site of Photoactive Yellow Protein. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5170-5178.	2.3	3
7955	The Decarboxylation of $\hat{1},\hat{2}$ -Unsaturated Acid Catalyzed by Prenylated FMN-Dependent Ferulic Acid Decarboxylase and the Enzyme Inhibition. <i>Journal of Organic Chemistry</i> , 2016, 81, 9289-9295.	1.7	25

#	ARTICLE	IF	CITATIONS
7956	Deleterious Effects of Exact Exchange Functionals on Predictions of Molecular Conductance. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3431-3435.	2.3	10
7957	N-Heterocyclic olefins as ancillary ligands in catalysis: a study of their behaviour in transfer hydrogenation reactions. <i>Dalton Transactions</i> , 2016, 45, 12835-12845.	1.6	37
7958	Experimental and theoretical analyses of ZnO nanoparticles deposited onto single-wall carbon nanotubes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2016, 24, 541-546.	1.0	1
7959	Electronic structure of SiO ₂ : An X-ray emission spectroscopic and density functional theoretical study. <i>Bulletin of the Russian Academy of Sciences: Physics</i> , 2016, 80, 738-741.	0.1	0
7960	Comprehensive DFT and TD-DFT Studies on the Photophysical Properties of 5,6-Dichloro-1,3-Bis(2-Pyridylimino)-4,7-Dihydroxyisoindole: A New Class of ESIPT Fluorophore. <i>Journal of Fluorescence</i> , 2016, 26, 1805-1812.	1.3	10
7961	Synthesis and Antiproliferative Activity of [RuCp(PPh ₃) ₂ (HdmoPTA)](OSO ₂ CF ₃) ₂ (HdmoPTA = 3,7-Dimethyl-1,3,7-triaza-5-phosphabicyclo[3.3.1]nonane). <i>Inorganic Chemistry</i> , 2016, 55, 7820-7822.	1.9	27
7962	Factors Controlling the Chemoselectivity in the Oxidation of Olefins by Nonheme Manganese(IV)-Oxo Complexes. <i>Journal of the American Chemical Society</i> , 2016, 138, 10654-10663.	6.6	52
7963	Role of para-substitution in controlling phosphatase activity of dinuclear Ni ^{II} complexes of Mannich-base ligands: experimental and DFT studies. <i>RSC Advances</i> , 2016, 6, 73534-73546.	1.7	8
7964	Spectroscopic and Computational Investigation of Low-spin Mn(III) Bis(scorpionate) Complexes. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 2413-2423.	1.0	13
7965	Synthesis and electronic structure determination of uranium(^{VI}) ligand radical complexes. <i>Dalton Transactions</i> , 2016, 45, 12576-12586.	1.6	30
7966	Solvatochromism, halochromism, and azo-hydrazone tautomerism in novel V-shaped azoazine colorants – consolidated experimental and computational approach. <i>Coloration Technology</i> , 2016, 132, 387-398.	0.7	13
7967	Phosphorescence or Thermally Activated Delayed Fluorescence? Intersystem Crossing and Radiative Rate Constants of a Three-Coordinate Copper(I) Complex Determined by Quantum-Chemical Methods. <i>Inorganic Chemistry</i> , 2016, 55, 7508-7516.	1.9	57
7968	Nondirected C-H Activation of Arenes with Cp*Ir(III) Acetate Complexes: An Experimental and Computational Study. <i>Organometallics</i> , 2016, 35, 2435-2445.	1.1	13
7969	Employing Range Separation on the meta-GGA Rung: New Functional Suitable for Both Covalent and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3662-3673.	2.3	10
7970	Vibrational averages along thermal lines. <i>Physical Review B</i> , 2016, 93, .	1.1	48
7971	Density functional theory study of the \pm phase transition in cerium: Role of electron correlation and orbital localization. <i>Physical Review B</i> , 2016, 93, .	1.1	23
7972	Reduced density-matrix functionals applied to the Hubbard dimer. <i>Physical Review B</i> , 2016, 93, .	1.1	20
7973	Uniaxial pressure-induced half-metallic ferromagnetic phase transition in LaMnO_3 . <i>Physical Review B</i> , 2016, 93, .	1.1	19

#	ARTICLE	IF	CITATIONS
7974	One- and many-electron self-interaction error in local and global hybrid functionals. <i>Physical Review B</i> , 2016, 93, .	1.1	62
7975	Ab initio charge-carrier mobility model for amorphous molecular semiconductors. <i>Physical Review B</i> , 2016, 93, .	1.1	46
7976	Tuning of the Electronic Levels of Oligothiophene–Naphthalimide Assemblies by Chemical Modification. <i>Chemistry - A European Journal</i> , 2016, 22, 13643-13652.	1.7	12
7977	Functional Conversion of CPD and (6–4) Photolyases by Mutation. <i>Biochemistry</i> , 2016, 55, 4173-4183.	1.2	20
7978	Theoretical Investigation of Structural Effects on the Charge Transfer Properties in Modified Phthalocyanines. <i>MRS Advances</i> , 2016, 1, 453-458.	0.5	1
7979	Dinuclear metal(II)-acetato complexes based on bicompartamental 4-chlorophenolate: syntheses, structures, magnetic properties, DNA interactions and phosphodiester hydrolysis. <i>Dalton Transactions</i> , 2016, 45, 12933-12950.	1.6	45
7980	[Al ₂ O ₄] ⁺ , a Benchmark Gas-Phase Class II Mixed-Valence Radical Anion for the Evaluation of Quantum-Chemical Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3796-3806.	2.3	20
7981	Enforcing the linear behavior of the total energy with hybrid functionals: Implications for charge transfer, interaction energies, and the random-phase approximation. <i>Physical Review B</i> , 2016, 94, .	1.1	52
7982	Why Replacing Different Oxygens of Thymine with Sulfur Causes Distinct Absorption and Intersystem Crossing. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6342-6350.	1.1	44
7983	Synthesis of enantiopure cyclopropyl esters from (–)-levoglucosenone. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 7520-7528.	1.5	17
7984	Effect of substitution on the ultrafast deactivation of the excited state of benzo[b]thiophene-arylamines. <i>Photochemical and Photobiological Sciences</i> , 2016, 15, 1029-1038.	1.6	8
7985	High-Performance All-Polymer Photoresponse Devices Based on Acceptor–Acceptor Conjugated Polymers. <i>Advanced Functional Materials</i> , 2016, 26, 6306-6315.	7.8	88
7986	Comparative QM/MM studies of H ₂ adsorption on lithium doped single walled armchair and zigzag nanotubes: SiCNT, GeCNT, and SnCNT. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1467-1476.	1.0	3
7987	The XYG3 type of doubly hybrid density functionals. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016, 6, 721-747.	6.2	52
7988	An acrylated isocyanonaphthalene based solvatochromic click reagent: Optical and biolabeling properties and quantum chemical modeling. <i>Dyes and Pigments</i> , 2016, 133, 445-457.	2.0	11
7989	Significant Influences of Elaborately Modulating Electron Donors on Light Absorption and Multichannel Charge-Transfer Dynamics for 4-(Benzo[<i>c</i>][1,2,5]thiadiazol-4-ylethynyl)benzoic Acid Dyes. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 18292-18300.	4.0	20
7990	Computational Assignment of the Histidine Protonation State in (6-4) Photolyase Enzyme and Its Effect on the Protonation Step. <i>ACS Catalysis</i> , 2016, 6, 5500-5507.	5.5	13
7991	A closer look on the coordination of soft nitrogen-donor ligands to Cm(III): SO ₃ -Ph-BTBP. <i>Dalton Transactions</i> , 2016, 45, 12308-12311.	1.6	7

#	ARTICLE	IF	CITATIONS
7992	Bi-anchoring Organic Dyes that Contain Benzimidazole Branches for Dye-Sensitized Solar Cells: Effects of π -Spacer and Peripheral Donor Groups. <i>Chemistry - an Asian Journal</i> , 2016, 11, 2564-2577.	1.7	32
7993	Trangmolins with an Unprecedented Structural Plasticity of the Rings A and B: New Insight into Limonoid Biosynthesis. <i>Chemistry - A European Journal</i> , 2016, 22, 11719-11727.	1.7	19
7994	molgw 1: Many-body perturbation theory software for atoms, molecules, and clusters. <i>Computer Physics Communications</i> , 2016, 208, 149-161.	3.0	139
7995	Charge transfer energies of benzene physisorbed on a graphene sheet from constrained density functional theory. <i>Physical Review B</i> , 2016, 93, .	1.1	13
7996	Relay-Like Exchange Mechanism through a Spin Radical between TbPc ₂ Molecules and Graphene/Ni(111) Substrates. <i>ACS Nano</i> , 2016, 10, 9353-9360.	7.3	26
7997	Can a Six-Letter Alphabet Increase the Likelihood of Photochemical Assault to the Genetic Code?. <i>Chemistry - A European Journal</i> , 2016, 22, 16648-16656.	1.7	17
7998	Performance of Hybrid DFT Compared to MP2 Methods in Calculating Nonlinear Optical Properties of Divinylpyrene Derivative Molecules. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8843-8852.	1.1	43
7999	Insights into the structural, electronic and magnetic properties of V-doped copper clusters: comparison with pure copper clusters. <i>Scientific Reports</i> , 2016, 6, 31978.	1.6	33
8000	Formation of the prebiotic molecule NH ₂ CHO on astronomical amorphous solid water surfaces: accurate tunneling rate calculations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29278-29285.	1.3	67
8001	First-principles study of structural and surface properties of (001) and (010) surfaces of hydroxylapatite and carbonated hydroxylapatite. <i>Journal of Applied Crystallography</i> , 2016, 49, 1893-1903.	1.9	22
8002	Alkenyl Arenes as Dipolarophiles in Catalytic Asymmetric 1,3-Dipolar Cycloaddition Reactions of Azomethine Ylides. <i>Angewandte Chemie</i> , 2016, 128, 15560-15564.	1.6	19
8003	Low-Temperature Disproportionation Reaction of NO on Au ₆ ⁺ : A Mechanism Involving Three NO Molecules Promoted by the Negative Charge. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9131-9137.	1.1	9
8004	Quantum chemical investigation on complexation of palladium with iminopyridyl ligands: Structural, thermochemical, and electronic aspects. <i>Molecular Crystals and Liquid Crystals</i> , 2016, 637, 53-64.	0.4	6
8005	Performance of DFT+U Approaches in the Study of Catalytic Materials. <i>ACS Catalysis</i> , 2016, 6, 8370-8379.	5.5	135
8006	Acquiring a record barrier height for magnetization reversal in lanthanide encapsulated fullerene molecules using DFT and ab initio calculations. <i>Chemical Communications</i> , 2016, 52, 14047-14050.	2.2	45
8007	Human Ferrochelatase: Insights for the Mechanism of Ferrous Iron Approaching Protoporphyrin IX by QM/MM and QTCP Free Energy Studies. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2421-2433.	2.5	14
8008	PbS Clusters Embedded in Sodalite Zeolite Cavities of Different Compositions: Unraveling the Structural Evolution and Optical Properties Using ab Initio Calculations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27050-27065.	1.5	12
8009	Alkenyl Arenes as Dipolarophiles in Catalytic Asymmetric 1,3-Dipolar Cycloaddition Reactions of Azomethine Ylides. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 15334-15338.	7.2	73

#	ARTICLE	IF	CITATIONS
8010	Restricted-Open-Shell G4(MP2)-Type Procedures. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9299-9304.	1.1	19
8011	Mechanistic aspects of the activation of C-H bond in C ₂ H ₆ by Th atom: bonding analysis and reaction coefficients. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	1
8012	Carbohydrate compounds as green corrosion inhibitors: electrochemical, XPS, DFT and molecular dynamics simulation studies. <i>RSC Advances</i> , 2016, 6, 110053-110069.	1.7	51
8013	In silico discovery of metal-organic frameworks for precombustion CO ₂ capture using a genetic algorithm. <i>Science Advances</i> , 2016, 2, e1600909.	4.7	231
8014	Oxidative DNA Cleavage Promoted by a Phenoxy-Radical Copper(II) Complex. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5575-5584.	1.0	4
8015	Enantioseparation of four amide herbicide stereoisomers using high-performance liquid chromatography. <i>Journal of Chromatography A</i> , 2016, 1471, 145-154.	1.8	26
8016	Failure of the IDA in FRET Systems at Close Inter-Dye Distances Is Moderated by Frequent Low $\langle \rho^2 \rangle$ Values. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8845-8862.	1.2	15
8017	Solvent-induced structural diversity in tetranuclear Ni(II) Schiff-base complexes: the first Ni ₄ single-molecule magnet with a defective dicubane-like topology. <i>Dalton Transactions</i> , 2016, 45, 18622-18634.	1.6	49
8018	Effect of Conjugation Pathway in Metal-Free Room-Temperature Dual Singlet-Triplet Emitters for Organic Light-Emitting Diodes. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4802-4808.	2.1	42
8019	Magnetic Circular Dichroism and Density Functional Theory Studies of Iron(II)-Pincer Complexes: Insight into Electronic Structure and Bonding Effects of Pincer N-Heterocyclic Carbene Moieties. <i>Organometallics</i> , 2016, 35, 3692-3700.	1.1	14
8020	Computational understanding of Li-ion batteries. <i>Npj Computational Materials</i> , 2016, 2, .	3.5	411
8021	Understanding the most favourable dimer of HCN for the oligomerization process in the gas phase of interstellar clouds. <i>Computational and Theoretical Chemistry</i> , 2016, 1097, 79-82.	1.1	6
8022	Quantum Chemical Calculations (Ab Initio & DFT), Hirshfeld Surface Analysis, Crystal Structure and Molecular Docking Study of 2-Chloro-4-(4-fluoro-phenyl)-6-isopropyl-pyrimidine-5-carboxylic Acid Methyl Ester. <i>Journal of Chemical Crystallography</i> , 2016, 46, 387-398.	0.5	7
8023	Experimental and Theoretical High-Energy-Resolution X-ray Absorption Spectroscopy: Implications for the Investigation of the Entatic State. <i>Inorganic Chemistry</i> , 2016, 55, 11694-11706.	1.9	25
8024	Investigation into Biological Environments through (Non)linear Optics: A Multiscale Study of Laurdan Derivatives. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6169-6181.	2.3	25
8025	Mechanistic implications of the enantioselective addition of alkylzinc reagents to aldehydes catalyzed by nickel complexes with β -amino amide ligands. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 11125-11136.	1.5	7
8026	Voltage and capacity control of polyaniline based organic cathodes: An ab initio study. <i>Journal of Power Sources</i> , 2016, 336, 126-131.	4.0	33
8027	Global reaction route mapping of water-catalysed gas phase oxidation of glyoxylic acid with hydroxyl radical. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	3

#	ARTICLE	IF	CITATIONS
8028	Copper(II) Complexes of Phenanthroline and Histidine Containing Ligands: Synthesis, Characterization and Evaluation of their DNA Cleavage and Cytotoxic Activity. <i>Inorganic Chemistry</i> , 2016, 55, 11801-11814.	1.9	66
8029	Assessment of quantum chemical methods for the calculation of homolytic N-H bond dissociation energies. <i>Chemical Data Collections</i> , 2016, 5-6, 28-35.	1.1	5
8030	Kinetics and Thermodynamics of Reversible Thiol Additions to Mono- and Diactivated Michael Acceptors: Implications for the Design of Drugs That Bind Covalently to Cysteines. <i>Journal of Organic Chemistry</i> , 2016, 81, 11726-11733.	1.7	106
8031	Device modeling challenges in the realm of overlapping physical scales: From atomistic to continuum, from coherent to diffusive transport. , 2016, , .		1
8032	Simulated Raman correlation spectroscopy for quantifying nucleic acid-silver composites. <i>Scientific Reports</i> , 2016, 6, 23535.	1.6	15
8033	Acridine-1, 8-diones – A new class of thermally stable NLOphores: Photophysical, (hyper)polarizability and TD-DFT studies. <i>Optical Materials</i> , 2016, 62, 306-319.	1.7	10
8034	Impact of the Alkyne Substitution Pattern and Metalation on the Photoisomerization of Azobenzene-Based Platinum(II) Diynes and Polyynes. <i>Inorganic Chemistry</i> , 2016, 55, 10955-10967.	1.9	19
8035	Does the DFT Self-Interaction Error Affect Energies Calculated in Proteins with Large QM Systems?. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5667-5679.	2.3	14
8036	Molybdenum dinitrogen complexes facially coordinated by linear tridentate PEP ligands (E = N or P): impact of the central E donor in trans-position to N ₂ . <i>Dalton Transactions</i> , 2016, 45, 14801-14813.	1.6	21
8037	Accurate description of hybridized local and charge-transfer excited-state in donor-acceptor molecules using density functional theory. <i>RSC Advances</i> , 2016, 6, 108404-108410.	1.7	23
8038	Beryllium-Based Anion Sponges: Close Relatives of Proton Sponges. <i>Chemistry - A European Journal</i> , 2016, 22, 18322-18325.	1.7	24
8039	Adsorption studies of NH ₃ molecules on functionalized germanene nanosheet – A DFT study. <i>Chemical Physics Letters</i> , 2016, 665, 22-30.	1.2	48
8040	A comparative molecular dynamics study of sulfuric and methanesulfonic acids. <i>Journal of Molecular Liquids</i> , 2016, 224, 1064-1073.	2.3	11
8041	Advances in Quantum Mechanochemistry: Electronic Structure Methods and Force Analysis. <i>Chemical Reviews</i> , 2016, 116, 14137-14180.	23.0	140
8042	Stille coupling via C-N bond cleavage. <i>Nature Communications</i> , 2016, 7, 12937.	5.8	87
8043	Benchmark tests of a strongly constrained semilocal functional with a long-range dispersion correction. <i>Physical Review B</i> , 2016, 94, .	1.1	152
8044	A computational investigation into the catalytic activity of a diselenolene sulfite oxidase biomimetic complex. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1127-1132.	0.6	5
8045	Nanocluster-Assembled Materials. <i>Series in Materials Science and Engineering</i> , 2016, , 113-148.	0.1	3

#	ARTICLE	IF	CITATIONS
8065	Porphyrin Analogues of a Trityl Cation and Anion. <i>Chemistry - A European Journal</i> , 2016, 22, 7041-7045.	1.7	8
8066	Efficient Preparation of TMS CCl_2 Br and Its Use in Dichlorocyclopropanation of Electron-Deficient Alkenes. <i>Chemistry - A European Journal</i> , 2016, 22, 7609-7616.	1.7	4
8067	Highly efficient implementation of pseudospectral time-dependent density-functional theory for the calculation of excitation energies of large molecules. <i>Journal of Computational Chemistry</i> , 2016, 37, 1425-1441.	1.5	29
8068	Induced Correspondence of a Local π -Aromatic Sextet in Heteroannulenes: Synthesis and Characterization. <i>Chemistry - A European Journal</i> , 2016, 22, 5504-5508.	1.7	6
8069	Aromatic Fused [30] Heteroannulenes with NIR Absorption and NIR Emission: Synthesis, Characterization, and Excited-State Dynamics. <i>Chemistry - A European Journal</i> , 2016, 22, 8026-8031.	1.7	11
8070	Ruthenium Complexes Containing 2,2'-bipyridine and 1,3,5-triaza-7-phosphaadamantane. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 1528-1540.	1.0	15
8071	The Valence States of Copernicium and Flerovium. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 2989-2992.	1.0	10
8072	NLOphoric Carbazole-Containing Push-Pull Extended Styryl Chromophores: Study of Photophysical Properties by Solvatochromic and DFT Method. <i>Journal of Fluorescence</i> , 2016, 26, 1261-1270.	1.3	5
8073	Structure and magnetic properties of Saturn-shaped fullerene complexes with ferrocene and nickelocene dicarboxylic acids: DFT simulation. <i>Structural Chemistry</i> , 2016, 27, 281-284.	1.0	3
8074	Empirical correction for PM7 band gaps of transition-metal oxides. <i>Journal of Molecular Modeling</i> , 2016, 22, 24.	0.8	0
8075	Enantioselective Synthesis of Polysubstituted Spiro-nitroprolinates Mediated by a (R,R)-Me-DuPhos-AgF-Catalyzed 1,3-Dipolar Cycloaddition. <i>Organic Letters</i> , 2016, 18, 2926-2929.	2.4	41
8076	Experimental and Theoretical Investigation for the Level of Conjugation in Carbazole-Based Precursors and Their Mono-, Di-, and Polynuclear Pt(II) Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 6465-6480.	1.9	24
8077	Dynamical Interactions of 5-Fluorouracil Drug with Dendritic Peptide Vectors: The Impact of Dendrimer Generation, Charge, Counterions, and Structured Water. <i>Journal of Physical Chemistry B</i> , 2016, 120, 5732-5743.	1.2	20
8078	A DFT+U study on the contribution of 4f electrons to oxygen vacancy formation and migration in Ln-doped CeO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 12938-12946.	1.3	43
8079	Thermoelectric properties of stannite-phase CuZn ₂ As ₄ (CZAS; A=Al, Ga and In) nanocrystals for solar energy conversion applications. <i>Philosophical Magazine</i> , 2016, 96, 2280-2299.	0.7	16
8080	Origin of Spectral Features and Acid-Base Properties of 3,7-Dihydroxyflavone and Its Monofunctional Derivatives in the Ground and Excited States. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4325-4337.	1.1	4
8081	Role of solvent in the phosphatase activity of a dinuclear nickel(Ni_2) complex of a Schiff base ligand: mechanistic interpretation by DFT studies. <i>New Journal of Chemistry</i> , 2016, 40, 7388-7398.	1.4	18
8082	Benzoylamido-substituted thiazoles and thiazolidines and their rhenium complexes. <i>Polyhedron</i> , 2016, 117, 293-299.	1.0	5

#	ARTICLE	IF	CITATIONS
8083	Surface selective binding of 2,5-dimercapto-1,3,4-thiadiazole (DMTD) on silver and gold nanoparticles: a Raman and DFT study. <i>RSC Advances</i> , 2016, 6, 62529-62539.	1.7	27
8084	Ground and Excited-Electronic-State Dissociations of Hydrogen-Rich and Hydrogen-Deficient Tyrosine Peptide Cation Radicals. <i>Journal of the American Society for Mass Spectrometry</i> , 2016, 27, 1454-1467.	1.2	15
8085	Tautomerism in substituted pyridofuroxans: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 105-111.	1.1	7
8086	Structure, vibrational analysis, electronic properties and chemical reactivity of two benzoxazole derivatives: Functional density theory study. <i>Journal of Molecular Structure</i> , 2016, 1123, 344-354.	1.8	18
8087	A Manganese(V)â€“Oxo Complex: Synthesis by Dioxygen Activation and Enhancement of Its Oxidizing Power by Binding Scandium Ion. <i>Journal of the American Chemical Society</i> , 2016, 138, 8523-8532.	6.6	118
8088	Geometric structure, electronic structure, and some thermodynamic properties of C13H22 trimethyl- and ethylmethyladamantanes. <i>Petroleum Chemistry</i> , 2016, 56, 166-170.	0.4	2
8089	Theoretical study on the structureâ€“property relationship of Dâ€“Aâ€“iâ€“A-type dye-sensitized solar cells: Î€-bridge and the side alkyl chain. <i>Canadian Journal of Chemistry</i> , 2016, 94, 794-801.	0.6	0
8090	â€œClickâ€•polymerization: A convenient strategy to prepare designer fullerene materials. <i>Materials and Design</i> , 2016, 108, 34-41.	3.3	16
8091	Toward unsaturated stannylenes Y ₂ ZrSn: and related compounds with triplet electronic ground states. <i>RSC Advances</i> , 2016, 6, 53749-53759.	1.7	4
8092	Isolation and Reactivity of Trifluoromethyl Iodonium Salts. <i>ACS Central Science</i> , 2016, 2, 341-350.	5.3	78
8093	Tuning the electronic and photophysical properties of platinum(II) complexes through ancillary ligand modification: a theoretical study. <i>Molecular Simulation</i> , 2016, 42, 1035-1041.	0.9	3
8094	Novel organoboron compounds derived from thieno[3,2-b]thiophene and triphenylamine units for OLED devices. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6045-6053.	2.7	53
8095	Thermolysis biradical mechanisms in endoperoxides: A challenge for density functional theory?. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	4
8096	Equilibrium and kinetic Si isotope fractionation factors and their implications for Si isotope distributions in the Earthâ€™s surface environments. <i>Acta Geochimica</i> , 2016, 35, 15-24.	0.7	24
8097	Hybrid Hamiltonian and Green's Function Approach for Studying Native Point Defect Levels in Semiconductor Compounds and Superlattices. <i>Journal of Electronic Materials</i> , 2016, 45, 4574-4579.	1.0	5
8098	Building high-coverage monolayers of covalently bound magnetic nanoparticles. <i>Applied Surface Science</i> , 2016, 388, 461-467.	3.1	17
8099	Spectroscopic and theoretical studies of some 4â€“substituted-phenyl 2-(ethanesulfonyl)acetates. Structure of 4â€“nitrophenyl 2-(ethanesulfonyl)acetate. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2016, 231, 23-34.	0.4	0
8100	Spectrometric measurements and DFT studies on new complex of copper (II) with		

#	ARTICLE	IF	CITATIONS
8101	Properties of two-dimensional insulators: A DFT study of bimetallic oxide CrW ₂ O ₉ clusters adsorption on MgO ultrathin films. <i>Applied Surface Science</i> , 2016, 379, 213-222.	3.1	5
8102	DFT investigation of NH ₃ gas interactions on TeO ₂ nanostructures. <i>Progress in Natural Science: Materials International</i> , 2016, 26, 129-138.	1.8	17
8103	Assignment of the absolute configuration at stereogenic phosphorus atoms in P-diastereomers of dithymidyl-(N ₃ â€²â†’P ₅ â€²)-phosphoramidothioate. <i>Tetrahedron</i> , 2016, 72, 803-809.	1.0	2
8104	Theoretical investigation on correlation between steric effects and selectivity in gasâ€²solid chlorination of polyvinyl chloride. <i>Chemical Engineering Science</i> , 2016, 151, 64-78.	1.9	6
8105	The mechanisms for triple gold(I)-catalyzed (4+1) cycloaddition of methylenecyclopropane with 7-naphthyl-1,3,5-cycloheptatriene: Insight into from density functional calculations. <i>Computational and Theoretical Chemistry</i> , 2016, 1084, 25-35.	1.1	7
8106	Tl(I) to Po(IV) 6s ² lone pairs in tetrahedral, triangular bipyramidal, square pyramidal, octahedral and hexahedral geometries: Crystal chemistry and ab initio visualizations and analyses. <i>Progress in Solid State Chemistry</i> , 2016, 44, 35-58.	3.9	9
8107	Molecular Investigation of the Mechanism of Non-Enzymatic Hydrolysis of Proteins and the Predictive Algorithm for Susceptibility. <i>Biochemistry</i> , 2016, 55, 3315-3328.	1.2	6
8108	The Complexation of Cm(III) with Succinate Studied by Time-Resolved Laser Fluorescence Spectroscopy and Quantum Chemical Calculations. <i>Inorganic Chemistry</i> , 2016, 55, 4504-4511.	1.9	7
8109	What roles do the residue Asp229 and the coordination variation of calcium play of the reaction mechanism of the diisopropyl-fluorophosphatase? A DFT investigation. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	9
8110	Polymorphism and Thermal Stability of Natural Active Ingredients. 3,3â€²-Diindolylmethane (Chemopreventive and Chemotherapeutic) Studied by a Combined X-ray, ¹ Hâ€² ¹⁴ N NMR-NQR, Differential Scanning Calorimetry, and Solid-State DFT/3D HS/QTAIM/RDS Computational Approach. <i>Crystal Growth and Design</i> , 2016, 16, 4336-4348.	1.4	9
8111	Structure, formation, thermodynamics and interactions in 9-carboxy-10-methylacridinium-based molecular systems. <i>New Journal of Chemistry</i> , 2016, 40, 7359-7372.	1.4	1
8112	<i>N</i> -Heterocyclic Carbene Capture by Cytochrome P450 3A4. <i>Molecular Pharmacology</i> , 2016, 90, 42-51.	1.0	7
8113	Biophysical Characterization of Fluorotyrosine Probes Site-Specifically Incorporated into Enzymes: <i>E. coli</i> Ribonucleotide Reductase As an Example. <i>Journal of the American Chemical Society</i> , 2016, 138, 7951-7964.	6.6	43
8114	Density function theoretical study on the complex involved in Th atom-activated Câ€²C bond in C ₂ H ₆ . <i>Chinese Physics B</i> , 2016, 25, 063102.	0.7	3
8115	Raman and XPS study on the interaction of taurine with silver nanoparticles. <i>RSC Advances</i> , 2016, 6, 56406-56411.	1.7	69
8116	Theoretical studies on the electronic structure and spectroscopic properties of transition metals <i>bis</i> (dipyrrinate)s. <i>Molecular Physics</i> , 2016, 114, 2838-2847.	0.8	3
8117	Electronic Circular Dichroism of [16]Helicene With Simplified TDâ€²DFT: Beyond the Single Structure Approach. <i>Chirality</i> , 2016, 28, 365-369.	1.3	30
8118	Nickel(II)â€²PPh ₃ Complexes of <i>S</i> , <i>N</i> -Substituted Thiosemicarbazones â€² Structure, DFT Study, and Catalytic Efficiency. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 538-544.	1.0	20

#	ARTICLE	IF	CITATIONS
8119	On the inclusion of post-MP2 contributions to double-hybrid density functionals. <i>Journal of Computational Chemistry</i> , 2016, 37, 183-193.	1.5	30
8120	QM/MM study of the interaction between zigzag SnC nanotube and small toxic gas molecules. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 411-420.	1.0	7
8121	Singlet Fission in Quinoidal Oligothiophenes. <i>Journal of Physical Chemistry C</i> , 2016, 120, 13901-13910.	1.5	28
8122	Transmetalation Process as a Route for Preparation of Zinc-Oxide-Supported Copper Nanoparticles. <i>Langmuir</i> , 2016, 32, 7029-7037.	1.6	9
8123	Second harmonic generation correlation spectroscopy for characterizing translationally diffusing protein nanocrystals. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 849-859.	1.1	1
8124	New sesquiterpenes and benzofuran derivatives from the aerial parts of <i>Asterothamnus centrali-asiaticus</i> . <i>Tetrahedron</i> , 2016, 72, 4910-4917.	1.0	6
8125	An Experimental and Theoretical Investigation on Pentacoordinated Cobalt(III) Complexes with an Intermediate $S=1$ Spin State: How Halide Ligands Affect their Magnetic Anisotropy. <i>Chemistry - A European Journal</i> , 2016, 22, 925-933.	1.7	21
8126	Theoretical Study of Pd ₁₁ Si ₆ Nanosheet Compounds Including Seven-Coordinated Si Species and Its Ge Analogues. <i>Chemistry - A European Journal</i> , 2016, 22, 1076-1087.	1.7	13
8127	Highly Convergent Synthesis of Intensively Blue Emissive Furo[2,3- <i>b</i>]isoquinolines by a Palladium-Catalyzed Cyclization Cascade of Unsaturated Ugi Products. <i>Chemistry - A European Journal</i> , 2016, 22, 2020-2031.	1.7	30
8128	Soluble Flavanthrone Derivatives: Synthesis, Characterization, and Application to Organic Light-Emitting Diodes. <i>Chemistry - A European Journal</i> , 2016, 22, 7978-7986.	1.7	15
8129	Interaction of arginine, lysine, and guanidine with surface residues of lysozyme: implication to protein stability. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 104-114.	2.0	21
8130	Photoredox catalysis for oxygenation/deoxygenation between sulfides and sulfoxides by visible-light-responsive polyoxometalates. <i>New Journal of Chemistry</i> , 2016, 40, 1014-1021.	1.4	46
8131	All-atom molecular dynamics simulations of an artificial sodium channel in a lipid bilayer: the effect of water solvation/desolvation of the sodium ion. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 529-539.	2.0	4
8132	Regio-selective synthesis of 5-substituted 1H-tetrazoles using ionic liquid [BMIM]N ₃ in solvent-free conditions: a click reaction. <i>Research on Chemical Intermediates</i> , 2016, 42, 1593-1610.	1.3	22
8133	Structures and Chemical Bonding in NbS _n (n = 3-5) Clusters: Effects of Sulfur Content and Charge States. <i>Journal of Cluster Science</i> , 2016, 27, 387-401.	1.7	3
8134	Problems, successes and challenges for the application of dispersion-corrected density-functional theory combined with dispersion-based implicit solvent models to large-scale hydrophobic self-assembly and polymorphism. <i>Molecular Simulation</i> , 2016, 42, 494-510.	0.9	13
8135	Structural Effects of the Donor Moiety on Reduction Kinetics of Oxidized Dye in Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3612-3618.	1.5	20
8136	Towards the origin of effective An(III)/Ln(III) separation by tridentate N-donor ligands: a theoretical study on atomic charges and polarisabilities for Cm(III)/Gd(III) separation. <i>Molecular Physics</i> , 2016, 114, 876-883.	0.8	19

#	ARTICLE	IF	CITATIONS
8137	Theoretical study on Pd-catalyzed reaction of aryl iodide with unsymmetrical alkyne. <i>Journal of Organometallic Chemistry</i> , 2016, 803, 134-141.	0.8	4
8138	Multifrequency cw-EPR and DFT Studies of an Apparent Compressed Octahedral Cu(II) Complex. <i>Inorganic Chemistry</i> , 2016, 55, 1497-1504.	1.9	16
8139	A Recyclable Organocatalyst for Asymmetric Michael Addition. <i>Catalysis Letters</i> , 2016, 146, 587-595.	1.4	4
8140	DFTB/PCM Applied to Ground and Excited State Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 2016, 120, 771-784.	1.1	16
8141	Rh ₂ (II,III) Catalysts with Chelating Carboxylate and Carboxamidate Supports: Electronic Structure and Nitrene Transfer Reactivity. <i>Journal of the American Chemical Society</i> , 2016, 138, 2327-2341.	6.6	95
8142	Type-I dyotropic rearrangement for 1,2-disubstituted cyclohexanes: substitution effect on activation energy. <i>RSC Advances</i> , 2016, 6, 10549-10556.	1.7	6
8143	Efficient Covalent Bond Formation in Gas-Phase Peptide-Peptide Ion Complexes with the Photoleucine Stapler. <i>Journal of the American Society for Mass Spectrometry</i> , 2016, 27, 633-645.	1.2	18
8144	Role of Heavy Atom Tunneling in Myers-Saito Cyclization of Cyclic Enyne-Cumulene Systems. <i>Journal of Physical Chemistry B</i> , 2016, 120, 945-950.	1.2	26
8145	Benzimidazole-thiazole based NLOphoric styryl dyes with solid state emission - Synthesis, photophysical, hyperpolarizability and TD-DFT studies. <i>Dyes and Pigments</i> , 2016, 128, 111-123.	2.0	36
8146	Improving the performance of dye-sensitized solar cells with electron-donor and electron-acceptor characteristic of planar electronic skeletons. <i>Energy and Environmental Science</i> , 2016, 9, 1390-1399.	15.6	71
8147	Direct ab initio study of the C ₆ H ₆ + CH ₃ /C ₂ H ₅ = C ₆ H ₅ + CH ₄ /C ₂ H ₆ reactions. <i>Chemical Physics Letters</i> , 2016, 646, 102-109.	1.2	9
8148	Pyrazole based NLOphores: Synthesis, photophysical, DFT, TDDFT studies. <i>Dyes and Pigments</i> , 2016, 127, 116-127.	2.0	30
8149	Theoretical Studies on Palladium-Mediated Enantioselective C-H Iodination. <i>Journal of Organic Chemistry</i> , 2016, 81, 1006-1020.	1.7	18
8150	Electronic structure and spectral properties of aurones as visible range fluorescent probes: a DFT/TDDFT study. <i>RSC Advances</i> , 2016, 6, 7002-7010.	1.7	28
8151	2,2-Bis(trifluoromethyl)biphenyl as a building block for highly ambient-stable, amorphous organic field-effect transistors with balanced ambipolarity. <i>RSC Advances</i> , 2016, 6, 8628-8638.	1.7	9
8152	Axial, Helical, and Planar Chirality in Directly Linked Basket-Handle Porphyrin Arrays. <i>Journal of Organic Chemistry</i> , 2016, 81, 1075-1088.	1.7	17
8153	Spectroscopic and Computational Investigations of The Thermodynamics of Boronate Ester and Diazaborole Self-Assembly. <i>Journal of Organic Chemistry</i> , 2016, 81, 969-980.	1.7	14
8154	Mechanism of thermal decomposition of 2-furyl radical. <i>Chemical Physics</i> , 2016, 465-466, 52-64.	0.9	7

#	ARTICLE	IF	CITATIONS
8155	Homojesterones: vinyllogous analogues of jesterone from <i>Helminthosporium velutinum</i> TS28. <i>Tetrahedron</i> , 2016, 72, 1031-1035.	1.0	9
8156	Theoretical Investigation of Adsorption, Dynamics, Self-Aggregation, and Spectroscopic Properties of the D102 Indoline Dye on an Anatase (101) Substrate. <i>Journal of Physical Chemistry C</i> , 2016, 120, 2787-2796.	1.5	23
8157	meso-Aryl-substituted free-base porphyrins: formation, structure and photostability of diprotonated species. <i>Research on Chemical Intermediates</i> , 2016, 42, 3789-3804.	1.3	11
8158	Novel NLOphoric 2-methoxy carbazole-based push pull chromophores: Synthesis, photophysical properties and TD-DFT Study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 321, 63-71.	2.0	23
8159	22 π -Electrons [1.1.1.1.1] pentaphyrin as a new photosensitizing agent for water disinfection: experimental and theoretical characterization. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	15
8160	Corrosion inhibition performance of pyranopyrazole derivatives for mild steel in HCl solution: Gravimetric, electrochemical and DFT studies. <i>Journal of Molecular Liquids</i> , 2016, 216, 78-86.	2.3	130
8161	Random phase approximation correlation energy using a compact representation for linear response functions: application to solids. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 035201.	0.7	8
8162	Indenocarbazole based bipolar host materials for highly efficient yellow phosphorescent organic light emitting diodes. <i>Organic Electronics</i> , 2016, 31, 11-18.	1.4	9
8163	Computational Design of a Family of Light-Driven Rotary Molecular Motors with Improved Quantum Efficiency. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 105-110.	2.1	67
8164	Isoskeletal Schiff base polynuclear coordination clusters: synthetic and theoretical aspects. <i>CrystEngComm</i> , 2016, 18, 704-713.	1.3	17
8165	Quantum chemical insight into the reactivity of 1,3-dipoles on coronene as model for nanographenes. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 173-182.	0.1	1
8166	Synthesis, NMR data and theoretical study of semi-synthetic derivatives from trans-dehydrocrotonin. <i>Journal of Molecular Structure</i> , 2016, 1108, 533-541.	1.8	2
8167	DFT and experimental studies on structure and spectroscopic parameters of 3,6-diiodo-9-ethyl-9H-carbazole. <i>Structural Chemistry</i> , 2016, 27, 199-207.	1.0	12
8168	Computational Studies of Bismuth-Doped Zinc Oxide Nanowires. <i>Nanoscience and Technology</i> , 2016, , 401-421.	1.5	1
8169	π -Donor-free π ™ oligo(3-hexylthiophene) dyes for efficient dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2016, 4, 2509-2516.	5.2	28
8170	A Molecular Chameleon with Fluorescein and Rhodamine Spectroscopic Behaviors. <i>Inorganic Chemistry</i> , 2016, 55, 205-213.	1.9	21
8171	Theoretical studies of the global minima and polarizabilities of small lithium clusters. <i>Chemical Physics Letters</i> , 2016, 644, 235-242.	1.2	13
8172	Electronically Excited States of Higher Acenes up to Nonacene: A Density Functional Theory/Multireference Configuration Interaction Study. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 305-312.	2.3	43

#	ARTICLE	IF	CITATIONS
8173	A novel C,D-spirodioxene taxoid synthesized through an unexpected Pd-mediated ring cyclization. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 345-352.	1.5	4
8174	Electrochemical, thermodynamic and quantum chemical studies of synthesized benzimidazole derivatives as corrosion inhibitors for N80 steel in hydrochloric acid. <i>Journal of Molecular Liquids</i> , 2016, 213, 122-138.	2.3	80
8175	First principles study of organic sensitizers for dye sensitized solar cells: effects of anchoring groups on optoelectronic properties and dye aggregation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1071-1081.	1.3	39
8176	A computationally efficient double hybrid density functional based on the random phase approximation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20926-20937.	1.3	55
8177	Theoretical and experimental studies of 1,5,7-triazabicyclo[4.4.0]dec-5-ene-catalyzed ring opening/ring closure reaction mechanism for 5-, 6- and 7-membered cyclic esters and carbonates. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2016, 117, 447-476.	0.8	20
8178	An amphoteric reactivity of a mixed-valent bis(μ -oxo)dimanganese(μ -oxo) complex acting as an electrophile and a nucleophile. <i>Dalton Transactions</i> , 2016, 45, 376-383.	1.6	24
8179	Solvent Polarity Tunes the Barrier Height for Twisted Intramolecular Charge Transfer in <i>N</i> -Pyrrolobenzonitrile (PBN). <i>Journal of Physical Chemistry A</i> , 2016, 120, 14-27.	1.1	15
8180	Synthesis and stereochemistry of new naphth[1,3]oxazino[3,2-a]benzazepine and naphth[1,3]oxazino[3,2-e]thienopyridine derivatives. <i>Tetrahedron</i> , 2016, 72, 2402-2410.	1.0	7
8181	Ethyl Nitroacetate in Aza-Henry Addition on Trifluoromethyl Aldimines: A Solvent-Free Procedure To Obtain Chiral Trifluoromethyl α,β -Diamino Esters. <i>Journal of Organic Chemistry</i> , 2016, 81, 2864-2874.	1.7	16
8182	Mechanistic and kinetic study on the reaction of ozone and trans-2-chlorovinyl dichloroarsine. <i>Chemosphere</i> , 2016, 150, 329-340.	4.2	2
8183	Novel 2H-pyran-3-carbonitrile dyes – Synthesis, solvatochromism study, and DFT, TD-DFT computations. <i>Journal of Luminescence</i> , 2016, 176, 298-308.	1.5	7
8184	Using the GVB Ansatz to develop ensemble DFT method for describing multiple strongly correlated electron pairs. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21040-21050.	1.3	22
8185	Molecular-Scale Electronics: From Concept to Function. <i>Chemical Reviews</i> , 2016, 116, 4318-4440.	23.0	1,014
8186	From Molecular Design to Co-sensitization; High performance indole based photosensitizers for dye-sensitized solar cells. <i>Electrochimica Acta</i> , 2016, 198, 10-21.	2.6	36
8187	Experimental, quantum chemical and Monte Carlo simulation studies of 3,5-disubstituted-4-amino-1,2,4-triazoles as corrosion inhibitors on mild steel in acidic medium. <i>Journal of Molecular Liquids</i> , 2016, 218, 281-293.	2.3	176
8188	New indole based co-sensitizers for dye sensitized solar cells exceeding 10% efficiency. <i>RSC Advances</i> , 2016, 6, 30205-30216.	1.7	34
8189	Coumarin Push-Pull NLOphores with Red Emission: Solvatochromic and Theoretical Approach. <i>Journal of Fluorescence</i> , 2016, 26, 949-962.	1.3	32
8190	[1]Benzothieno[3,2- <i>b</i>]benzothiophene-Based Organic Dyes for Dye-Sensitized Solar Cells. <i>Journal of Organic Chemistry</i> , 2016, 81, 3235-3245.	1.7	52

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8191	1,1,4,4-Tetracyanobuta-1,3-diene Substituted Diketopyrrolopyrroles: An Acceptor for Solution Processable Organic Bulk Heterojunction Solar Cells. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6324-6335.	1.5	61
8192	Connectivity matters – ultrafast isomerization dynamics of bisazobenzene photoswitches. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14795-14804.	1.3	69
8193	Electronic structure of transition metal ions in GaN and AlN: Comparing GGA+U with experiment. <i>Journal of Alloys and Compounds</i> , 2016, 664, 565-579.	2.8	25
8194	Acetate bridged dinuclear Cu(II) complexes with ferrocene based benzimidazol ligands: Synthesis, spectroscopy, electrochemistry, DFT calculations and catecholase activity. <i>Polyhedron</i> , 2016, 111, 109-117.	1.0	6
8195	Predicting the Efficiency of Photoswitches Using Force Analysis. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1298-1302.	2.1	11
8196	The molecular mechanism of palladium-catalysed cyanoesterification of methyl cyanofornate onto norbornene. <i>Dalton Transactions</i> , 2016, 45, 7786-7793.	1.6	9
8197	Heats of formation of platonic hydrocarbon cages by means of high-level thermochemical procedures. <i>Journal of Computational Chemistry</i> , 2016, 37, 49-58.	1.5	66
8198	Puckering Energetics and Optical Activities of [7]Circulene Conformers. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1074-1083.	1.1	18
8199	Structural and magnetic properties of heptacoordinated Mn ^{II} complexes containing a 15-membered pyridine-based macrocycle and halido/pseudohalido axial coligands. <i>RSC Advances</i> , 2016, 6, 34674-34684.	1.7	17
8200	X-Band Electron Paramagnetic Resonance Comparison of Mononuclear Mn ^{IV} -oxo and Mn ^{IV} -hydroxo Complexes and Quantum Chemical Investigation of Mn ^{IV} Zero-Field Splitting. <i>Inorganic Chemistry</i> , 2016, 55, 3272-3282.	1.9	27
8201	Exploring the limits of recent exchange-correlation functionals in modeling lithium/benzene interaction. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	26
8202	Fine-tuning of a radical-based reaction by radical <i>S</i> -adenosyl-L-methionine tryptophan lyase. <i>Science</i> , 2016, 351, 1320-1323.	6.0	53
8203	Enantioselective endocrine disrupting effects of omeprazole studied in the H295R cell assay and by molecular modeling. <i>Toxicology in Vitro</i> , 2016, 34, 71-80.	1.1	13
8204	Thienylphenothiazine integrated pyrenes: an account on the influence of substitution patterns on their optical and electroluminescence properties. <i>Journal of Materials Chemistry C</i> , 2016, 4, 4246-4258.	2.7	33
8205	Metal nanoparticle catalyzed charge rearrangement in selenourea probed by surface-enhanced Raman scattering. <i>RSC Advances</i> , 2016, 6, 17405-17414.	1.7	33
8206	A novel donor-acceptor carbazole and benzothiadiazole material for deep red and infrared emitting applications. <i>Journal of Materials Chemistry C</i> , 2016, 4, 2219-2227.	2.7	40
8207	Predicting ¹⁷ O NMR chemical shifts of polyoxometalates using density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8235-8241.	1.3	4
8208	¹³ C Bond Cleavage of Zinc-Polyhistidine Complexes in Electron Transfer Dissociation Mediated by Zwitterion Formation: Experimental Evidence and Theoretical Analysis of the Utah-Washington Model. <i>Journal of Physical Chemistry B</i> , 2016, 120, 891-901.	1.2	10

#	ARTICLE	IF	CITATIONS
8209	Geometrical structure of meta-xylylene based symmetric polyradicals and their magnetic nature: A density functional study. <i>Chemical Physics Letters</i> , 2016, 648, 189-194.	1.2	3
8210	Computing UV/vis spectra using a combined molecular dynamics and quantum chemistry approach: bis-triazin-pyridine (BTP) ligands studied in solution. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7728-7736.	1.3	21
8211	Self-Assembly of Tetraphenyldibenzoperiflanthene (DBP) Films on Ag(111) in the Monolayer Regime. <i>Langmuir</i> , 2016, 32, 1981-1987.	1.6	18
8212	The stereoselectivities of tributyltin hydride-mediated reductions of 5-bromo- <i>d</i> -glucuronides to <i>l</i> -iduronides are dependent on the anomeric substituent: syntheses and DFT calculations. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 2950-2960.	1.5	12
8213	Ionisation and (de-)protonation energies of gas-phase amino acids from an optimally tuned range-separated hybrid functional. <i>Molecular Physics</i> , 2016, 114, 1218-1224.	0.8	11
8214	Experimental and Computational Studies on the Reactivity and Binding Mode of Thiophene with N-Heterocyclic Carbene Iridium Complexes. <i>Organometallics</i> , 2016, 35, 569-578.	1.1	4
8215	Unusual Electrochemical Properties of the Electropolymerized Thin Layer Based on a <i>i</i> -Tetrazine-Triphenylamine Monomer. <i>Journal of Physical Chemistry C</i> , 2016, 120, 4382-4391.	1.5	28
8216	Effects of central metal on electronic structure, magnetic properties, infrared and Raman spectra of double-decker phthalocyanine. <i>Applied Surface Science</i> , 2016, 380, 127-134.	3.1	12
8217	Formation, Characterization, and O=O Bond Activation of a Peroxomanganese(III) Complex Supported by a Cross-Clamped Cyclam Ligand. <i>Inorganic Chemistry</i> , 2016, 55, 2055-2069.	1.9	27
8218	Electrochromic behaviour of triazine based ambipolar compounds. <i>Electrochimica Acta</i> , 2016, 192, 283-295.	2.6	23
8219	Gauging the Performance of Density Functionals for Lanthanide-Containing Molecules. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1259-1266.	2.3	39
8220	Gauge effects in local hybrid functionals evaluated for weak interactions and the GMTKN30 test set. <i>Molecular Physics</i> , 2016, 114, 1118-1127.	0.8	26
8221	Proton Mobility in b_2 Ion Formation and Fragmentation Reactions of Histidine-Containing Peptides. <i>Journal of the American Society for Mass Spectrometry</i> , 2016, 27, 487-497.	1.2	18
8222	Mechanistic investigation of palladium-catalyzed amidation of aryl halides. <i>Journal of Molecular Modeling</i> , 2016, 22, 53.	0.8	6
8223	Structure and Properties of Zirconia Nanoparticles from Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 4392-4402.	1.5	85
8224	Aerobic oxidative cyclization of benzamides via meta-selective C-H tert-alkylation: rapid entry to 7-alkylated isoquinolinediones. <i>Chemical Communications</i> , 2016, 52, 4470-4473.	2.2	62
8225	Metanephrine neuroendocrine tumor marker detection by SERS using Au nanoparticle/Au film sandwich architecture. <i>Biomedical Microdevices</i> , 2016, 18, 12.	1.4	11
8226	Insulating oxide surfaces and nanostructures. <i>Comptes Rendus Physique</i> , 2016, 17, 471-480.	0.3	7

#	ARTICLE	IF	CITATIONS
8227	Transnitrosylation products of the dipeptide cysteinyl-L-cysteine: an examination by tandem mass spectrometry and density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6047-6052.	1.3	3
8228	Manipulation of carbon nanotube magnetism with metal-rich iron nanoparticles. <i>Journal of Materials Chemistry C</i> , 2016, 4, 1215-1227.	2.7	7
8229	How large are post-CCSD(T) contributions to the total atomization energies of medium-sized alkanes?. <i>Chemical Physics Letters</i> , 2016, 645, 118-122.	1.2	12
8230	A study of oligothiophene acceptor dyes in p-type dye-sensitized solar cells. <i>RSC Advances</i> , 2016, 6, 18165-18177.	1.7	21
8231	Amorphous Protic Ionic Systems as Promising Active Pharmaceutical Ingredients: The Case of the Sumatriptan Succinate Drug. <i>Molecular Pharmaceutics</i> , 2016, 13, 1111-1122.	2.3	15
8232	Polymorphism and disorder in natural active ingredients. Low and high-temperature phases of anhydrous caffeine: Spectroscopic (^1H - ^{14}N NMR/NQR/ ^{14}N NQR) and solid-state computational modelling (DFT/QTAIM/RDS) study. <i>European Journal of Pharmaceutical Sciences</i> , 2016, 85, 18-30.	1.9	14
8233	Boron-doped hydrogenated Al ₃ clusters: A material for hydrogen storage. <i>Journal of Alloys and Compounds</i> , 2016, 667, 275-281.	2.8	26
8234	Radical Monocationic Guanidino-Functionalized Aromatic Compounds (GFAs) as Bridging Ligands in Dinuclear Metal Acetate Complexes: Synthesis, Electronic Structure, and Magnetic Coupling. <i>Inorganic Chemistry</i> , 2016, 55, 1683-1696.	1.9	25
8235	A comparative study of novel chalcone derivative by X-ray and quantum chemical calculations (Ab-initio and DFT): Experimental and theoretical approach. <i>Molecular Crystals and Liquid Crystals</i> , 2016, 624, 190-204.	0.4	16
8236	Anti-corrosive properties of 4-amino-3,5-bis(disubstituted)-1,2,4-triazole derivatives on mild steel corrosion in 2 M H ₃ PO ₄ solution: Experimental and theoretical studies. <i>Journal of Molecular Liquids</i> , 2016, 216, 874-886.	2.3	76
8237	Influence of Electron Correlation on the Electronic Structure and Magnetism of Transition-Metal Phthalocyanines. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1772-1785.	2.3	54
8238	Using the general-purpose reactivity indicator: challenging examples. <i>Journal of Molecular Modeling</i> , 2016, 22, 57.	0.8	5
8239	Polyoxometalate-based nanozyme: Design of a multifunctional enzyme for multi-faceted treatment of Alzheimer's disease. <i>Nano Research</i> , 2016, 9, 1079-1090.	5.8	96
8240	Dehydrohalogenation Condensation Reaction of Phenylhydrazine with Cl-Terminated Si(111) Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 5539-5548.	1.5	12
8241	Two-State Reactivity in Low-Valent Iron-Mediated C-H Activation and the Implications for Other First-Row Transition Metals. <i>Journal of the American Chemical Society</i> , 2016, 138, 3715-3730.	6.6	136
8242	Synthesis and characterization of thieno[3,4-d]imidazole-based organic sensitizers for photoelectrochemical cells. <i>Dyes and Pigments</i> , 2016, 129, 60-70.	2.0	10
8243	Electronic Structure of a Cu ^{II} -Alkoxide Complex Modeling Intermediates in Copper-Catalyzed Alcohol Oxidations. <i>Journal of the American Chemical Society</i> , 2016, 138, 4132-4145.	6.6	12
8244	Optimizing link atom parameters for DNA QM/MM simulations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	5

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8245	Crystal solvates of zinc(II) bis(dipyrrinates) with triethylamine: composition, stability and spectral-luminescent properties. <i>Journal of Coordination Chemistry</i> , 2016, 69, 901-914.	0.8	9
8246	Understanding anionic Chugaev elimination in pericyclic tetracene formation. <i>Tetrahedron</i> , 2016, 72, 1686-1689.	1.0	3
8247	Excited-State Proton-Transfer-Induced Trapping Enhances the Fluorescence Emission of a Locked GFP Chromophore. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 753-764.	2.3	44
8248	Connection between Hybrid Functionals and Importance of the Local Density Approximation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1605-1612.	1.1	13
8249	Kohn-Sham calculations of NMR shifts for paramagnetic 3d metal complexes: protocols, delocalization error, and the curious amide proton shifts of a high-spin iron(II) macrocycle complex. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21051-21068.	1.3	37
8250	Electronic, bonding, linear and non-linear optical properties of novel Li ₂ Ga ₂ GeS ₆ compound. <i>Journal of Alloys and Compounds</i> , 2016, 674, 109-115.	2.8	9
8251	On the applicability of hybrid functionals for predicting fundamental properties of metals. <i>Solid State Communications</i> , 2016, 234-235, 10-13.	0.9	36
8252	Alkoxycarbonylation of $\hat{1}\pm, \hat{1}^2$ -unsaturated amides catalyzed by palladium(II) complexes: a DFT study of the mechanism. <i>RSC Advances</i> , 2016, 6, 8440-8448.	1.7	6
8253	Decomposition of the fluoroethylene carbonate additive and the glue effect of lithium fluoride products for the solid electrolyte interphase: an ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8643-8653.	1.3	118
8254	The HO ₂ + (H ₂ O) _n + O ₃ reaction: an overview and recent developments. <i>European Physical Journal D</i> , 2016, 70, 1.	0.6	11
8255	Charge generation in organic photovoltaics: a review of theory and computation. <i>Molecular Systems Design and Engineering</i> , 2016, 1, 10-24.	1.7	86
8256	The S66x8 benchmark for noncovalent interactions revisited: explicitly correlated ab initio methods and density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20905-20925.	1.3	182
8257	Raman and infrared spectra, normal coordinate analysis and ab initio calculations of 4-Amino-2-chloropyrimidine-5-carbonitrile. <i>Journal of Molecular Structure</i> , 2016, 1115, 85-93.	1.8	6
8258	A systematic study on Pt based, subnanometer-sized alloy cluster catalysts for alkane dehydrogenation: effects of intermetallic interaction. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10906-10917.	1.3	29
8259	DFT Studies on Interaction of H ₂ S Gas with $\hat{1}\pm$ -Fe ₂ O ₃ Nanostructures. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2016, 26, 394-404.	1.9	28
8260	A series of new heteroleptic Hg(II) complexes: Synthesis, crystal structures and photophysical properties. <i>Polyhedron</i> , 2016, 110, 131-141.	1.0	11
8261	Electronic Structure Evolution during the Growth of Graphene Nanoribbons on Au(110). <i>Journal of Physical Chemistry C</i> , 2016, 120, 7323-7331.	1.5	16
8262	Mechanism of Rh ₂ (II)-Catalyzed Indole Formation: The Catalyst Does Not Control Product Selectivity. <i>Journal of the American Chemical Society</i> , 2016, 138, 487-490.	6.6	53

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8263	Liquid-liquid equilibria for ternary mixtures of water+ 2-propanol+ 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquids at 298.15 K. <i>Fluid Phase Equilibria</i> , 2016, 412, 205-210.	1.4	59
8264	Predicting Near Edge X-ray Absorption Spectra with the Spin-Free Exact-Two-Component Hamiltonian and Orthogonality Constrained Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 144-156.	2.3	42
8265	Oxidation of phenyl and hydride ligands of bis(pentamethylcyclopentadienyl)hafnium derivatives by nitrous oxide via selective oxygen atom transfer reactions: insights from quantum chemistry calculations. <i>Dalton Transactions</i> , 2016, 45, 1152-1159.	1.6	6
8266	What Are the Ground State Structures of C ₂₀ and C ₂₄ ? An Explicitly Correlated Ab Initio Approach. <i>Journal of Physical Chemistry A</i> , 2016, 120, 153-160.	1.1	51
8267	In vivo detection of fluoride at trace levels and its removal from raw water at neutral pH utilizing a cyanobacterium pigment as a luminescent probe. <i>RSC Advances</i> , 2016, 6, 4410-4421.	1.7	4
8268	Cyclopentadienone Oxidation Reaction Kinetics and Thermochemistry for the Alcohols, Hydroperoxides, and Vinylic, Alkoxy, and Alkylperoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2016, 120, 433-451.	1.1	12
8269	Synthesis, reactions and DFT calculations of novel bis(chalcones) linked to a thienothiophene core through an oxyphenyl bridge. <i>RSC Advances</i> , 2016, 6, 10949-10961.	1.7	17
8270	Calculation of low bandgap homopolymers: Comparison of TD-DFT methods with experimental oligomer series. <i>Chemical Physics Letters</i> , 2016, 645, 169-173.	1.2	26
8271	Exploring the low-lying structures of Au _n (CO) _{n+1} (n = 1-10): adsorption and stretching frequencies of CO on various coordination sites. <i>RSC Advances</i> , 2016, 6, 8248-8255.	1.7	4
8272	Butadiene dyes based on 3-(dicyanomethylidene)indan-1-one and 1,3-bis(dicyanomethylidene)indane: synthesis, characterization and solvatochromic behaviour. <i>RSC Advances</i> , 2016, 6, 6858-6867.	1.7	11
8273	Benchmark <i>ab Initio</i> Conformational Energies for the Proteinogenic Amino Acids through Explicitly Correlated Methods. Assessment of Density Functional Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 444-454.	2.3	99
8274	Copper(II) quinolinonato-7-carboxamido complexes as potent antitumor agents with broad spectra and selective effects. <i>RSC Advances</i> , 2016, 6, 3899-3909.	1.7	23
8275	Kinetic and structural studies reveal a unique binding mode of sulfite to the nickel center in urease. <i>Journal of Inorganic Biochemistry</i> , 2016, 154, 42-49.	1.5	42
8276	Predictive modelling of the LD50 activities of coumarin derivatives using neural statistical approaches: Electronic descriptor-based DFT. <i>Journal of Taibah University for Science</i> , 2016, 10, 451-461.	1.1	8
8277	Nucleophilicity and P=C Bond Formation Reactions of a Terminal Phosphanido Iridium Complex. <i>Inorganic Chemistry</i> , 2016, 55, 828-839.	1.9	9
8278	$\text{I}^4\text{-Oxo}$ stabilized by three metal cations is a sufficient nucleophile for enzymatic hydrolysis of phosphate monoesters. <i>Dalton Transactions</i> , 2016, 45, 2517-2522.	1.6	6
8279	H-Bond Isomerization in Crystalline Cellulose III _I : Proton Hopping versus Hydroxyl Flip-Flop. <i>ACS Macro Letters</i> , 2016, 5, 50-54.	2.3	9
8280	Nanoscale cross-correlated AFM, Kelvin probe, elastic modulus and quantum mechanics investigation of clay mineral surfaces: The case of chlorite. <i>Applied Clay Science</i> , 2016, 131, 175-181.	2.6	30

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8281	Theoretical study of electron transport properties of bimolecular junctions: Effect of molecular arrangement and species. <i>Computational Materials Science</i> , 2016, 113, 53-59.	1.4	6
8282	Electronic structure, magnetic and optical properties of Cr-doped GaAs using hybrid density functional. <i>Computational Materials Science</i> , 2016, 113, 75-79.	1.4	7
8283	Protonated thiophene-based oligomers as formed within zeolites: understanding their electron delocalization and aromaticity. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2080-2086.	1.3	17
8284	Theoretical study on fluorescent probes for cyanide based on the indolium functional group. <i>Organic Electronics</i> , 2016, 30, 1-11.	1.4	8
8285	Density functional theory study on the magnetic properties of Co ₃ O ₄ with normal spinel structure. <i>Journal of Physics and Chemistry of Solids</i> , 2016, 91, 86-89.	1.9	11
8286	Near-infrared unsymmetrical blue and green squaraine sensitizers. <i>Photochemical and Photobiological Sciences</i> , 2016, 15, 287-296.	1.6	19
8287	Molecular and electronic structure of 1,3,2-diazaphosphinine derivatives. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2016, 191, 399-404.	0.8	2
8288	Influence of structural factors and the properties of the medium on the fluorescence of Zn(II) bis(dipyrrinate)s. <i>Journal of Luminescence</i> , 2016, 170, 275-281.	1.5	8
8289	Host-guest complexation of di-cyclohexanocucurbit[6]uril and hexa-cyclohexanocucurbit[6]uril with alkyldiammonium ions: a comparative study. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 674-679.	1.5	17
8290	Pyrazole based solid state emissive NLOphores with TICT characteristics: Synthesis, DFT and TDDFT studies. <i>Dyes and Pigments</i> , 2016, 126, 62-75.	2.0	38
8291	Unusual Fluorescent Responses of Morpholine-Functionalized Fluorescent Probes to pH via Manipulation of BODIPY's HOMO and LUMO Energy Orbitals for Intracellular pH Detection. <i>ACS Sensors</i> , 2016, 1, 158-165.	4.0	82
8292	Experimental and theoretical evidences of the influence of hydrogen bonding on the catalytic activity of a series of 2-hydroxy substituted quaternary ammonium salts in the styrene oxide/CO ₂ coupling reaction. <i>Journal of Catalysis</i> , 2016, 333, 29-39.	3.1	66
8293	Pyrolysis reaction networks for lignin model compounds: unraveling thermal deconstruction of ̂ ² -O-4 and ̂ [±] -O-4 compounds. <i>Green Chemistry</i> , 2016, 18, 1762-1773.	4.6	92
8294	Prediction of binding modes and affinities of 4-substituted-2,3,5,6-tetrafluorobenzenesulfonamide inhibitors to the carbonic anhydrase receptor by docking and ONIOM calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 63, 38-48.	1.3	15
8295	Exploring the structural and conformational properties of dioxygen dihalides (halogen = F, Cl, Br). <i>Canadian Journal of Chemistry</i> , 2016, 94, 176-187.	0.6	4
8296	Ferrocenyl-substituted dinuclear Cu(II) complex: Synthesis, spectroscopy, electrochemistry, DFT calculations and catecholase activity. <i>Journal of Molecular Structure</i> , 2016, 1106, 331-342.	1.8	5
8297	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 332-344.	2.3	42
8298	Analysis of creatine phosphate disodium salt by ESI-MS/MS: A seven-centered rearrangement mechanism in gas phase. <i>International Journal of Mass Spectrometry</i> , 2016, 394, 42-45.	0.7	1

#	ARTICLE	IF	CITATIONS
8299	A computational study of lithium interaction with tetracyanoethylene (TCNE) and tetracyaniquinodimethane (TCNQ) molecules. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1470-1477.	1.3	32
8300	Unlocking the effects of ancillary electron-donors on light absorption and charge recombination in phenanthrocarbazole dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2016, 4, 519-528.	5.2	31
8301	Promising Strategy To Improve Charge Separation in Organic Photovoltaics: Installing Permanent Dipoles in PCBM Analogues. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4664-4671.	1.1	30
8302	Aggregation induced emissive carbazole-based push pull NLOphores: Synthesis, photophysical properties and DFT studies. <i>Dyes and Pigments</i> , 2016, 124, 82-92.	2.0	46
8303	Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. <i>Molecular Physics</i> , 2016, 114, 21-33.	0.8	21
8304	High-affinity selective inhibitor against phospholipase A ₂ (PLA ₂): a computational study. <i>Journal of Receptor and Signal Transduction Research</i> , 2016, 36, 111-118.	1.3	5
8305	Comparison of Relative Activation Energies Obtained by Density Functional Theory and the Random Phase Approximation for Several Claisen Rearrangements. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1486-1496.	1.2	10
8306	Electronic and optical properties of Mg-, F-doped and Mg ²⁺ -F-codoped M _{1-VO} 2 via hybrid density functional calculations. <i>Journal of Alloys and Compounds</i> , 2016, 658, 569-575.	2.8	30
8308	Computational Chemistry of Catalytic Biomass Conversion. <i>Green Chemistry and Sustainable Technology</i> , 2016, , 63-104.	0.4	0
8309	Photophysics of Auramine-O: electronic structure calculations and nonadiabatic dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 403-413.	1.3	15
8310	Effective chemiluminogenic systems based on acridinium esters bearing substituents of various electronic and steric properties. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 652-668.	1.5	19
8311	A novel method for the calculation of bond stretching force constants of diatomic molecules. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 154, 103-107.	2.0	12
8312	Electrostatic and stereoelectronic interaction impacts on the structural properties and isomerization reactions of methyl isocyanide and its trihalo-analogs. <i>Structural Chemistry</i> , 2016, 27, 883-896.	1.0	4
8313	How Anion Chaotrope Changes the Local Structure of Water: Insights from Photoelectron Spectroscopy and Theoretical Modeling of SCN ⁻ Water Clusters. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1518-1525.	1.2	20
8314	A Density Functional Theory Investigation of the Tandem Radical Cyclization of 1-[2-Yl-3-(2-Methoxyphenyl)-prop-2-enyl]-6-oxo-1,6-dihydropyridine-2-carbonitrile. <i>Australian Journal of Chemistry</i> , 2016, 69, 319.	0.5	2
8315	The effect of hydrogen bond strength on emission properties in 2-(2-hydroxyphenyl)imidazo[1,2-a]pyridines. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 314, 198-213.	2.0	17
8316	Efficient and tunable phosphorescence of new platinum(II) complexes based on the donor-acceptor Schiff bases. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 316, 12-18.	2.0	17
8317	Electronic Structure of Crystalline Buckyballs: fcc-C60. <i>Journal of Electronic Materials</i> , 2016, 45, 339-348.	1.0	26

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8318	Using DFT Methods to Study Activators in Optical Materials. <i>ECS Journal of Solid State Science and Technology</i> , 2016, 5, R3007-R3018.	0.9	31
8319	Fluorescent difluoroboron-curcumin analogs: An investigation of the electronic structures and photophysical properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 152, 241-251.	2.0	47
8320	Synthesized amino acid compounds as eco-friendly corrosion inhibitors for mild steel in hydrochloric acid solution: electrochemical and quantum studies. <i>Research on Chemical Intermediates</i> , 2016, 42, 2641-2660.	1.3	34
8321	Inter- and intramolecular C-H...O interactions on aliphatic and cyclohexane carbonyl derivatives. <i>Journal of Computational Chemistry</i> , 2016, 37, 25-33.	1.5	17
8322	Global and local interactions in the structure of crystalline 7-(diethylamino)-2-(2-oxo-2H-chromen-3-yl)chromenium perchlorate. <i>Structural Chemistry</i> , 2016, 27, 637-649.	1.0	2
8323	Isolation and characterization of bioactive compounds of <i>Clematis gouriana</i> Roxb. ex DC against snake venom phospholipase A ₂ (PLA ₂) computational and <i>in vitro</i> insights. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 1936-1949.	2.0	11
8324	l-Histidinium thiocyanurate: Experimental and theoretical studies of a new nonlinear optical material. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 172, 168-173.	2.0	1
8325	Structural and nonlinear optical studies of a salt with an octupolar chromophore: Guanidinium cyclopropanecarboxylate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 172, 156-162.	2.0	9
8326	Numerical simulation and a parametric study of inorganic nanowire solar cells. <i>International Journal of Numerical Modelling: Electronic Networks, Devices and Fields</i> , 2017, 30, e2176.	1.2	3
8327	Complete ¹ H NMR assignment of cedranolides. <i>Magnetic Resonance in Chemistry</i> , 2017, 55, 169-176.	1.1	13
8328	Insights into the Thermal Eliminations and Photoeliminations of B,N-Heterocycles: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 753-761.	1.1	9
8329	Cross C-S coupling reaction catalyzed by copper(<i>scpi</i>) N-heterocyclic carbene complexes. <i>RSC Advances</i> , 2017, 7, 4912-4920.	1.7	24
8330	Theoretical investigation and molecular docking approach on the antioxidant activity of Schiff bases and their tautomers. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750001.	1.8	3
8331	Plasma polymerization of poly(3,4-ethylenedioxyethene) films: The influence of plasma gas phase chemistry. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2017, 35, .	0.9	8
8332	Investigations on the frontier orbitals of FeFn (n=1-6) superhalogen complexes and prediction of novel salt series Li-(FeFn). <i>Journal of Fluorine Chemistry</i> , 2017, 195, 85-92.	0.9	9
8333	Understanding Local Defects in Li-Ion Battery Electrodes through Combined DFT/NMR Studies: Application to LiVPO ₄ F. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3219-3227.	1.5	37
8334	Density functional theory is straying from the path toward the exact functional. <i>Science</i> , 2017, 355, 49-52.	6.0	711
8335	Low and High Molecular Mass Dithienopyrrole-Naphthalene Bisimide Donor-Acceptor Compounds: Synthesis, Electrochemical and Spectroelectrochemical Behaviour. <i>Chemistry - A European Journal</i> , 2017, 23, 2839-2851.	1.7	14

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8336	Comprehensive study on excited state intramolecular proton transfer in 2-(benzo[d]thiazol-2-yl)-3-methoxynaphthalen-1-ol and 2-(benzo[d]thiazol-2-yl)naphthalene-1,3-diol: Effect of solvent, aggregation, viscosity and TDDFT study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 337, 33-43.	2.0	15
8337	Nonadiabatic photodynamics and UV absorption spectrum of all-trans-octatetraene. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3937-3947.	1.3	9
8338	Molecular engineering of Dâ€“Aâ€“Iâ€“A sensitizers for highly efficient solid-state dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2017, 5, 3157-3166.	5.2	41
8339	Ligand-Field-Dependent Behavior of Meta-GGA Exchange in Transition-Metal Complex Spin-State Ordering. <i>Journal of Physical Chemistry A</i> , 2017, 121, 874-884.	1.1	52
8340	TD-DFT Study of Absorption and Emission Spectra of 2-(2â€“Aminophenyl)benzothiazole Derivatives in Water. <i>Journal of Fluorescence</i> , 2017, 27, 745-754.	1.3	7
8341	Substituent and Solvent Effects on the Stability of <i>N</i> -Heterocyclic Carbene Complexes with CO ₂ . <i>Journal of Organic Chemistry</i> , 2017, 82, 1552-1557.	1.7	38
8342	Inhibition effect of E and Z conformations of 2-pyridinealdazine on mild steel corrosion in phosphoric acid. <i>Anti-Corrosion Methods and Materials</i> , 2017, 64, 23-35.	0.6	14
8343	Comparative theoretical and experimental study on novel tri-quinoline system and its anticancer studies. <i>Journal of Molecular Structure</i> , 2017, 1134, 770-780.	1.8	7
8344	Copper(I) Complexes Bearing 1,2-Phenyl-Bridged P ³ N, P ³ N ³ P, and N ³ P ³ N Chelate Ligands: Structures and Phosphorescence. <i>Inorganic Chemistry</i> , 2017, 56, 1616-1625.	1.9	56
8345	New Insight into the Formation Mechanism of Imidazolium-Based Ionic Liquids from <i>N</i> -Alkyl Imidazoles and Halogenated Hydrocarbons: A Polar Microenvironment Induced and Autopromoted Process. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1133-1139.	1.1	9
8346	Absorption Tails of Donor:C ₆₀ Blends Provide Insight into Thermally Activated Charge-Transfer Processes and Polaron Relaxation. <i>Journal of the American Chemical Society</i> , 2017, 139, 1699-1704.	6.6	73
8347	Unusual binding modes in the copper(ii) and palladium(ii) complexes of peptides containing both histidyl and cysteinyl residues. <i>New Journal of Chemistry</i> , 2017, 41, 1372-1379.	1.4	8
8348	The optoelectronic properties of new dyes based onâ€“thienopyrazine. <i>Comptes Rendus Chimie</i> , 2017, 20, 461-466.	0.2	22
8349	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. <i>Chemistry of Materials</i> , 2017, 29, 1964-1988.	3.2	116
8350	Reducing density-driven error without exact exchange. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4793-4801.	1.3	19
8351	Anions coordinating anions: analysis of the interaction between anionic Keplerate nanocapsules and their anionic ligands. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5343-5350.	1.3	7
8352	Bonding trends across the series of tricarbonato-actinyl anions [(AnO ₂)(CO ₃) ₃] ⁴⁻ (An = Uâ€“Cm): the plutonium turn. <i>Dalton Transactions</i> , 2017, 46, 2542-2550.	1.6	34
8353	Interaction of phenolic acids with trypsin: Experimental and molecular modeling studies. <i>Food Chemistry</i> , 2017, 228, 1-6.	4.2	34

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8354	Stable isotope fractionation of tungsten during adsorption on Fe and Mn (oxyhydr)oxides. <i>Geochimica Et Cosmochimica Acta</i> , 2017, 204, 52-67.	1.6	56
8355	Computational Studies on Rhodium(III) Catalyzed C-H Functionalization versus Deoxygenation of Quinoline N-Oxides with Diazo Compounds. <i>Organometallics</i> , 2017, 36, 650-656.	1.1	19
8356	The first examples of multiply bonded dirhenium($\text{Rhenium}^{\text{III}}$, $\text{Rhenium}^{\text{II}}$) paramagnetic complexes containing nitrobenzoate ligands: spectroscopic, structural, cytotoxicity and computational studies. <i>Dalton Transactions</i> , 2017, 46, 5670-5679.	1.6	9
8357	Deposition of copper from Cu^{I} and Cu^{II} precursors onto HOPG surface: Role of surface defects and choice of a precursor. <i>Journal of Chemical Physics</i> , 2017, 146, 052814.	1.2	16
8358	Weak Intermolecular Interactions: A Supramolecular Approach. , 2017, , 593-619.		4
8359	Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2017, , 795-860.		6
8360	Directions for Use of Density Functional Theory: A Short Instruction Manual for Chemists. , 2017, , 225-267.		2
8361	Stability, and optical and electronic properties of ultrathin h-BNC. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5629-5636.	1.3	24
8362	Study of adiabatic connection in density functional theory with an accurate wavefunction for two-electron spherical systems. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25344.	1.0	6
8363	Excitation spectra of Ag ⁺ -DNA bases complexes: A benchmark study. <i>Chemical Physics Letters</i> , 2017, 673, 11-18.	1.2	15
8364	DFT/TD-DFT characterization of conjugational electronic structures and spectral properties of materials based on thieno[3,2-b][1]benzothiophene for organic photovoltaic and solar cell applications. <i>Journal of Saudi Chemical Society</i> , 2017, 21, 563-574.	2.4	44
8365	Modulation of the L_a/L_b Mixing in an Indole Derivative: A Position-Dependent Study Using 4-, 5-, and 6-Fluoroindole. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1597-1606.	1.1	12
8366	Triphenylamine-Based Fluorescent Styryl Dyes: DFT, TD-DFT and Non-Linear Optical Property Study. <i>Journal of Fluorescence</i> , 2017, 27, 993-1007.	1.3	21
8367	Computational exploration of regioselectivity and atmospheric lifetime in NO ₃ -initiated reactions of CH ₃ OCH ₃ and CH ₃ OCH ₂ CH ₃ . <i>Journal of Molecular Graphics and Modelling</i> , 2017, 72, 156-167.	1.3	3
8368	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 679-695.	2.3	19
8369	Dissecting the Cytochrome P450 1A2- and 3A4-Mediated Metabolism of Aflatoxin B1 in Ligand and Protein Contributions. <i>Chemistry - A European Journal</i> , 2017, 23, 2884-2893.	1.7	31
8370	Extension of the ReaxFF Combustion Force Field toward Syngas Combustion and Initial Oxidation Kinetics. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1051-1068.	1.1	204
8371	Conformational analysis of a modified RGD adhesive sequence. <i>Journal of Peptide Science</i> , 2017, 23, 172-181.	0.8	2

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8372	Spectroelectrochemistry of alternating ambipolar copolymers of 4,4'- and 2,2'-bipyridine isomers and quaterthiophene. <i>Electrochimica Acta</i> , 2017, 231, 437-452.	2.6	12
8373	Synthesis, characterization, X-ray crystallography and stability in aqueous medium of trans-[Ru(CO)(NH ₃) ₄ P(OH) ₃] ²⁺ . <i>Polyhedron</i> , 2017, 124, 184-190.	1.0	2
8374	Enhancing and optimizing electronic transport in biphenyl derivative single-molecule junctions attached to carbon nanotubes electrodes. <i>Solid State Communications</i> , 2017, 252, 46-50.	0.9	1
8375	Electrochemically Induced Synthesis of Triphenylamine-based Polyhydrazones. <i>Electrochimica Acta</i> , 2017, 230, 10-21.	2.6	29
8376	Adsorption of Sulfonamides on Phyllosilicate Surfaces by Molecular Modeling Calculations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2905-2914.	1.5	23
8377	Correlation of the structural information obtained for europium-chelate ensembles from gas-phase photoluminescence and ion-mobility spectroscopy with density-functional computations and ligand-field theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6105-6112.	1.3	7
8378	From cadmium(II)-aroylhydrazone complexes to metallopolymers with enhanced photoluminescence. A structural and DFT study. <i>Inorganica Chimica Acta</i> , 2017, 458, 129-137.	1.2	29
8379	Atmospheric fate of diketones and OH radical kinetics, reaction force, ETS-NOCV analysis. <i>Molecular Physics</i> , 2017, 115, 839-859.	0.8	9
8380	Singularity Correction for Long-Range-Corrected Density Functional Theory with Plane-Wave Basis Sets. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2035-2045.	1.1	1
8381	Development of New Density Functional Approximations. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 155-182.	4.8	51
8382	Calculations of solid-state ⁴³ Ca NMR parameters: A comparison of periodic and cluster approaches and an evaluation of DFT functionals. <i>Journal of Computational Chemistry</i> , 2017, 38, 949-956.	1.5	19
8383	The screened pseudo-charge repulsive potential in perturbed orbitals for band calculations by DFT+U. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8008-8025.	1.3	40
8384	White Light from a Single Fluorophore: A Strategy Utilizing Excited-State Intramolecular Proton-Transfer Phenomenon and Its Verification. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5277-5286.	1.5	38
8385	S-Functionalization of 3,5-bis(2-pyridyl)-1,2,4,6-thiatriazine: probing the effect of alkyl chain length in the development of tethered materials. <i>New Journal of Chemistry</i> , 2017, 41, 2268-2276.	1.4	1
8386	Characterization of a Dinuclear Copper(II) Complex and Its Fleeting Mixed-Valent Copper(II)/Copper(III) Counterpart. <i>ChemPlusChem</i> , 2017, 82, 615-624.	1.3	9
8387	Theoretical study on the mechanism of the N ₂ H ₄ plus O ₂ reaction on the singlet and triplet potential energy surfaces. <i>Computational and Theoretical Chemistry</i> , 2017, 1104, 47-55.	1.1	3
8388	Adaptively Compressed Exchange Operator for Large-Scale Hybrid Density Functional Calculations with Applications to the Adsorption of Water on Silicene. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1188-1198.	2.3	38
8389	Effect of molecular structure on spin-dependent electron transport in biferrocene-based molecular junctions: a first-principles study. <i>Journal of Computational Electronics</i> , 2017, 16, 340-346.	1.3	11

#	ARTICLE	IF	CITATIONS
8390	Is a 1,4-Alkyl Shift Involved in the Biosynthesis of Ledol and Viridiflorol?. <i>Journal of Organic Chemistry</i> , 2017, 82, 3957-3959.	1.7	10
8391	Zirconocene-Based Methods for the Preparation of BN-Indenes: Application to the Synthesis of 1,5-Dibora-4a,8a-diaza-1,2,3,5,6,7-hexaaryl-4,8-dimethyl- <i>indacenes</i> . <i>Organometallics</i> , 2017, 36, 2541-2551.	1.1	24
8392	Gas-phase COS activation by U+: Reaction mechanisms and bonding analysis. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750010.	1.8	0
8393	First hyperpolarizability of cyclooctatetraene modulated by alkali and alkaline earth metals. <i>Journal of Molecular Modeling</i> , 2017, 23, 93.	0.8	7
8394	Theoretical approaches for predicting the color of rigid dyes in solution. <i>Journal of Computational Chemistry</i> , 2017, 38, 998-1004.	1.5	17
8395	Effects of donor position on dibenzofulvene-based organic dyes for photovoltaics. <i>Journal of Materials Science: Materials in Electronics</i> , 2017, 28, 8694-8707.	1.1	8
8396	Chemiluminogenic acridinium salts: A comparison study. Detection of intermediate entities appearing upon light generation. <i>Journal of Luminescence</i> , 2017, 187, 102-112.	1.5	14
8397	Significant electron transfer in heme catalysis: The case of chlorite dismutase. <i>Journal of Catalysis</i> , 2017, 348, 40-46.	3.1	11
8398	Donor-acceptor conjugated copolymers incorporating tetrafluorobenzene as the electron deficient unit. <i>Journal of Polymer Science Part A</i> , 2017, 55, 1601-1610.	2.5	20
8399	Photostability of Coumarin Laser Dyes - a Mechanistic Study Using Global and Local Reactivity Descriptors. <i>Journal of Fluorescence</i> , 2017, 27, 1101-1108.	1.3	31
8400	Origin of the Regioselectivity in the Aldol Condensation between Hydroxymethylfurfural and Levulinic Acid: A DFT Investigation. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1985-1992.	1.1	6
8401	Solvatomorphs of 25,26,27,28-tetrahydroxycalix[4]arene and 5,11,17,23-tetramino-25,26,27,28-tetrabutoxycalix[4]arene: quenching photoluminescence through switching the guest. <i>CrystEngComm</i> , 2017, 19, 1792-1800.	1.3	5
8402	Revisiting the hydration structure of aqueous Na+. <i>Journal of Chemical Physics</i> , 2017, 146, 084504.	1.2	90
8403	Two novel thorium organic frameworks constructed by bi- and tritopic ligands. <i>Radiochimica Acta</i> , 2017, 105, 531-539.	0.5	1
8404	Modeling adsorbate-induced property changes of carbon nanotubes. <i>Journal of Computational Chemistry</i> , 2017, 38, 861-868.	1.5	3
8405	Monolayer of Hydrazine Facilitates the Direct Covalent Attachment of C ₆₀ Fullerene to a Silicon Surface. <i>Langmuir</i> , 2017, 33, 8632-8639.	1.6	10
8406	Dynamic quantum crystallography: lattice-dynamical models refined against diffraction data. II. Applications to L-alanine, naphthalene and xylitol. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, 102-114.	0.0	23
8407	Interpolated energy densities, correlation indicators and lower bounds from approximations to the strong coupling limit of DFT. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6169-6183.	1.3	28

#	ARTICLE	IF	CITATIONS
8408	Reaching across the Divide: How Monometalation of One Binding Pocket Affects the Empty Binding Pocket in a Siamese-Twin Porphyrin Palladium Complex. <i>Inorganic Chemistry</i> , 2017, 56, 2221-2232.	1.9	3
8409	One Lump or Two? A Plurality of Pathways in Gold(III)-Catalyzed Cyclization Transforming Propargyl Acetates to a Carene-like Bicyclo[4.1.0]heptane. <i>Organometallics</i> , 2017, 36, 920-926.	1.1	6
8410	Ion Effect and Metal-Coordinated Cross-Linking for Multiscale Design of Nereis Jaw Inspired Mechanomutable Materials. <i>ACS Nano</i> , 2017, 11, 1858-1868.	7.3	24
8411	An integrated flow microcalorimetry, infrared spectroscopy and density functional theory approach to the study of chromate complexation on hematite and ferrihydrite. <i>Chemical Geology</i> , 2017, 464, 23-33.	1.4	26
8412	Fingerprints of Through-Bond and Through-Space Exciton and Charge π -Electron Delocalization in Linearly Extended [2.2]Paracyclophanes. <i>Journal of the American Chemical Society</i> , 2017, 139, 3095-3105.	6.6	34
8413	Exploring the possibility to store the mixed oxygen-hydrogen cluster in clathrate hydrate in molar ratio 1:2 (O ₂ + 2H ₂). <i>Journal of Molecular Graphics and Modelling</i> , 2017, 73, 1-7.	1.3	2
8414	Sensing properties of monolayer borophane nanosheet towards alcohol vapors: A first-principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 73, 208-216.	1.3	37
8415	Asymmetric hydrogen bonding in formic acid π -nitric acid dimer observed by quantum molecular dynamics simulations. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	2
8416	Identification of Al ₁₃ on the Colloid Surface Using Surface-Enhanced Raman Spectroscopy. <i>Environmental Science & Technology</i> , 2017, 51, 2899-2906.	4.6	13
8417	Synthesis of Novel Thiazole Based Carbaldehyde as Potential Sensor for Fluoride Anion and their Spectroscopic Properties. <i>Journal of Fluorescence</i> , 2017, 27, 1117-1128.	1.3	10
8418	Redox Control of Aluminum Ring-Opening Polymerization: A Combined Experimental and DFT Investigation. <i>Macromolecules</i> , 2017, 50, 1847-1861.	2.2	56
8419	Iridium π -NSiN catalyzed formation of silylphosphinecarboxylates from the reaction of CO ₂ with P(SiMe ₃) ₃ R ₂ (R = Ph, Cy). <i>Catalysis Science and Technology</i> , 2017, 7, 1372-1378.	2.1	6
8420	Modeling organic electronic materials: bridging length and time scales. <i>Molecular Simulation</i> , 2017, 43, 730-742.	0.9	8
8421	Innovative Carbon Dioxide π Capturing Organic Solvent: Reaction Mechanism and Kinetics. <i>Chemical Engineering and Technology</i> , 2017, 40, 737-744.	0.9	8
8422	[Cu(H ₂ O) _n] ²⁺ (n=6) complexes in solution phase: a DFT hierarchical study. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	18
8423	A theoretical study on oxidative cleavage of olefins to carbonyls catalysed by Fe(π -PyBisulidine). <i>Dalton Transactions</i> , 2017, 46, 3825-3832.	1.6	3
8424	Rapidly accessible π -rotaxanes utilizing a single amide hydrogen bond templating motif. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 2797-2803.	1.5	15
8425	Accurate alkynyl radical structures from density functional calculations without Hartree-Fock exchange. <i>Journal of Chemical Physics</i> , 2017, 146, 054109.	1.2	5

#	ARTICLE	IF	CITATIONS
8426	Structure-Activity Relationship To Screen Ni-Bisphosphine Complexes for the Oxidative Coupling of CO ₂ and Ethylene. <i>Organometallics</i> , 2017, 36, 1107-1112.	1.1	19
8427	When does a functional correctly describe both the structure and the energy of the transition state?. <i>Journal of Molecular Modeling</i> , 2017, 23, 65.	0.8	5
8428	Microwave dielectric relaxation spectroscopy study of propylene glycol/ethanol binary mixtures: Temperature dependence. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 179, 74-82.	2.0	21
8429	Molecular and thin film properties of cobalt half-sandwich compounds for optoelectronic application. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6768-6776.	1.3	9
8430	Modifying electronic properties of ICBA through chemical substitutions for solar cell applications. <i>Structural Chemistry</i> , 2017, 28, 1133-1140.	1.0	6
8431	Calculations of current densities for neutral and doubly charged persubstituted benzenes using effective core potentials. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7124-7131.	1.3	43
8432	Sulfate radical oxidation of aromatic contaminants: a detailed assessment of density functional theory and high-level quantum chemical methods. <i>Environmental Sciences: Processes and Impacts</i> , 2017, 19, 395-404.	1.7	48
8433	Density Functional Theory: Not Quite the Right Answer for the Right Reason Yet. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 5396-5398.	7.2	45
8434	Small Nonplanar Phenothiazine-oxide-Based Molecules: Structural Characterization, Photophysical, Thermal and Computational Studies. <i>ChemistrySelect</i> , 2017, 2, 3084-3092.	0.7	12
8435	Tuning the Fe(II/III) Redox Potential in Nonheme Fe(II)-Hydroxo Complexes through Primary and Secondary Coordination Sphere Modifications. <i>Inorganic Chemistry</i> , 2017, 56, 4852-4863.	1.9	35
8436	Benchmarking the GW Approximation and Bethe-Salpeter Equation for Groups IB and IIB Atoms and Monoxides. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2135-2146.	2.3	34
8437	A quantum chemical study on [•] Cl-initiated atmospheric degradation of acrylonitrile. <i>RSC Advances</i> , 2017, 7, 20574-20581.	1.7	3
8438	En route towards the peptide β -helix: X-ray diffraction analyses and conformational energy calculations of Adm-rich short peptides. <i>Journal of Peptide Science</i> , 2017, 23, 346-362.	0.8	8
8439	Au ₁₀ (SG) ₁₀ : A Chiral Gold Catenane Nanocluster with Zero Confined Electrons. Optical Properties and First-Principles Theoretical Analysis. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1979-1985.	2.1	49
8440	Potassium <i>tert</i> -Butoxide-Catalyzed Dehydrogenative C-H Silylation of Heteroaromatics: A Combined Experimental and Computational Mechanistic Study. <i>Journal of the American Chemical Society</i> , 2017, 139, 6867-6879.	6.6	160
8441	Synthesis and characterization of a dipyrriamethyrin-uranyl complex. <i>Chemical Communications</i> , 2017, 53, 4981-4984.	2.2	27
8442	Impact of Halogenido Coligands on Magnetic Anisotropy in Seven-Coordinate Co(II) Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 5076-5088.	1.9	57
8443	Bowl-shaped structures from acylphloroglucinols: an <i>ab initio</i> and DFT study. <i>Molecular Physics</i> , 2017, 115, 2254-2266.	0.8	11

#	ARTICLE	IF	CITATIONS
8444	The atmospheric oxidation of CH ₃ OOH by the OH radical: the effect of water vapor. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12331-12342.	1.3	28
8445	Correcting density-driven errors in projection-based embedding. <i>Journal of Chemical Physics</i> , 2017, 146, 084113.	1.2	14
8446	First-Principles Insights of CO Adsorption Characteristics on Ge and In Substituted Silicene Nanosheet. <i>Silicon</i> , 2017, 9, 327-337.	1.8	18
8447	On the decay of the triplet state of thionucleobases. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12674-12682.	1.3	38
8448	Electronic, optical and magnetic properties of Co, Fe and Ni doped (ZnX) ₆ ; (X = O, S & Se) quantum dots – A DFT study. <i>Computational and Theoretical Chemistry</i> , 2017, 1111, 56-68.	1.1	6
8449	QTAIM and NCI analysis of intermolecular interactions in steroid ligands binding a cytochrome P450 enzyme – Beyond the most obvious interactions. <i>Computational and Theoretical Chemistry</i> , 2017, 1111, 40-49.	1.1	24
8450	Synthesis, characterization and phosphatase inhibitory activity of dioxidovanadium(V) complexes with Schiff base ligands derived from pyridoxal and resorcinol. <i>Polyhedron</i> , 2017, 130, 184-194.	1.0	13
8451	From nitrogen inversion in amines to stereoinversion in aminium salts: role of a single water molecule. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	5
8452	Chemical Protection of Material Morphology: Robust and Gentle Gas-Phase Surface Functionalization of ZnO with Propiolic Acid. <i>Chemistry of Materials</i> , 2017, 29, 4063-4071.	3.2	16
8453	Effect of Fluoride Modification on the Phillips Cr/SiO ₂ Catalyst for Ethylene Polymerization. <i>ChemCatChem</i> , 2017, 9, 3364-3373.	1.8	9
8454	The role of the long-range exchange corrections in the description of electron delocalization in aromatic species. <i>Journal of Computational Chemistry</i> , 2017, 38, 1640-1654.	1.5	69
8455	Cu ⁰ -catalysed 1,3-dipolar cycloadditions of α -amino acid derived N,N-cyclic azomethine imines to ynones. <i>Tetrahedron</i> , 2017, 73, 3329-3337.	1.0	10
8456	Furfural: The Unimolecular Dissociative Photoionization Mechanism of the Simplest Furanic Aldehyde. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3401-3410.	1.1	8
8457	Mechanisms of Carbonyl Activation by BINOL <i>N</i> -Triflylphosphoramides: Enantioselective Nazarov Cyclizations. <i>ACS Catalysis</i> , 2017, 7, 3466-3476.	5.5	25
8458	Electronic structure investigation of biphenylene films. <i>Journal of Chemical Physics</i> , 2017, 146, 054705.	1.2	16
8459	Decomposition of Effective Exchange Integrals of Radical Dimers Using Bond Energy Density Analysis. <i>Chemistry Letters</i> , 2017, 46, 879-882.	0.7	1
8460	From NAD ⁺ to Nickel Pincer Complex: A Significant Cofactor Evolution Presented by Lactate Racemase. <i>Chemistry - A European Journal</i> , 2017, 23, 7545-7557.	1.7	20
8461	Comparing the performance of TD-DFT and SAC-CI methods in the description of excited states potential energy surfaces: An excited state proton transfer reaction as case study. <i>Journal of Computational Chemistry</i> , 2017, 38, 1084-1092.	1.5	15

#	ARTICLE	IF	CITATIONS
8462	Electronic g Tensors in U^V Complexesâ€“A Computational Study. Chemistry - A European Journal, 2017, 23, 7798-7808.	1.7	4
8463	Electronic relaxation pathways of the biologically relevant pterin chromophore. Physical Chemistry Chemical Physics, 2017, 19, 12720-12729.	1.3	11
8464	New trace of secondary organic aerosol from oxidation of acetonitrile with radical hydroxyl. Computational and Theoretical Chemistry, 2017, 1113, 72-81.	1.1	5
8465	A study of asymmetrical mixed-valent Mo₂â€“Mo₂ complexes in the class III regime. Dalton Transactions, 2017, 46, 5711-5723.	1.6	6
8466	First principle calculation of accurate native defect levels in CaF2. European Physical Journal B, 2017, 90, 1.	0.6	6
8467	Effect of anion and alkyl chain length on the structure and interactions of N -alkyl pyridinium ionic liquids. Journal of Molecular Liquids, 2017, 240, 694-707.	2.3	31
8468	Benchmark Relative Energies for Large Water Clusters with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2017, 13, 2696-2704.	2.3	34
8469	Coumarin-Pyrazole Hybrid with Red Shifted ESIPT Emission and AIE Characteristics - a Comprehensive Study. Journal of Fluorescence, 2017, 27, 1687-1707.	1.3	15
8470	What Makes a Density Functional Approximation Good? Insights from the Left Fukui Function. Journal of Chemical Theory and Computation, 2017, 13, 2373-2377.	2.3	33
8471	First-Principle Study on the Effect of Pi-Spacers on Small Molecule Acceptors: Quantum Design of Organic Solar Cells and NLO Compounds. Journal of Cluster Science, 2017, 28, 2419-2431.	1.7	5
8472	Efficacy of Density Functionals and Relativistic Effective Core Potentials for Lanthanide-Containing Species: The Ln54 Molecule Set. Journal of Chemical Theory and Computation, 2017, 13, 2831-2839.	2.3	25
8473	Atropisomerism and Conformational Equilibria: Impact on PI3KÍ Inhibition of 2-((6-Amino-9<i>H</i>-purin-9-yl)methyl)-5-methyl-3-(<i>o</i>-tolyl)quinazolin-4(3<i>H</i>)-one (IC87114) and Its Conformationally Restricted Analogs. Journal of Medicinal Chemistry, 2017, 60, 4304-4315.	2.9	15
8474	Navigating Past a Fork in the Road: Carbocationâ€“Î€ Interactions Can Manipulate Dynamic Behavior of Reactions Facing Post-Transition-State Bifurcations. Journal of the American Chemical Society, 2017, 139, 7485-7493.	6.6	51
8475	Nucleation of Small Silicon Carbide Dust Clusters in AGB Stars. Astrophysical Journal, 2017, 840, 117.	1.6	32
8476	Theoretical investigation of the photochromic properties of [2.2]paracyclophane-bridged imidazole dimers and bis(imidazole) dimers. Tetrahedron, 2017, 73, 4936-4949.	1.0	8
8477	Conformation of repaglinide: A solvent dependent structure. Journal of Molecular Structure, 2017, 1143, 388-396.	1.8	7
8478	Exploring the reaction channels between arsine and the hydroxyl radical. Molecular Physics, 2017, 115, 2431-2441.	0.8	3
8479	Synthesis of Structurally Complex Silicon Frameworks through the First Silaâ€“Aldol Reaction. Angewandte Chemie - International Edition, 2017, 56, 8089-8093.	7.2	8

#	ARTICLE	IF	CITATIONS
8480	Molecular structure, second- and third-order nonlinear optical properties and DFT studies of a novel non-centrosymmetric chalcone derivative: (2E)-3-(4-fluorophenyl)-1-(4-(((1E)-(4-fluorophenyl)methylene)amino)phenyl)prop-2-en-1-one. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 184, 342-354.	2.0	74
8481	Design of diblock co-oligomers as low bandgap small molecules for organic solar cells. <i>Molecular Simulation</i> , 2017, 43, 1496-1501.	0.9	3
8482	Synthesis of Structurally Complex Silicon Frameworks through the First Sila-aldol Reaction. <i>Angewandte Chemie</i> , 2017, 129, 8201-8205.	1.6	4
8483	Cobalt complexes based on 2-(1H-benzimidazol-2-yl)-phenol derivatives: preparation, spectral studies, DFT calculations and catalytic behavior toward ethylene oligomerization. <i>Journal of Coordination Chemistry</i> , 2017, 70, 1800-1814.	0.8	6
8484	Nacre-inspired design of graphene oxide-polydopamine nanocomposites for enhanced mechanical properties and multi-functionalities. <i>Nano Futures</i> , 2017, 1, 011003.	1.0	41
8485	Four faces of the interaction between ions and aromatic rings. <i>Journal of Computational Chemistry</i> , 2017, 38, 1762-1773.	1.5	9
8486	The Effect of the cis-donor in pincer ligands on hydrogenolysis of Pd-OH: A DFT study. <i>Journal of Organometallic Chemistry</i> , 2017, 845, 165-170.	0.8	4
8487	Importance of MM Polarization in QM/MM Studies of Enzymatic Reactions: Assessment of the QM/MM Drude Oscillator Model. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2954-2961.	2.3	34
8488	Controlling the Conductance of a Graphene-Molecule Nanojunction by Proton Transfer. <i>Nano Letters</i> , 2017, 17, 3341-3346.	4.5	15
8489	Aggregation and Dissociation of Aqueous Al ₁₃ Induced by Fluoride Substitution. <i>Environmental Science & Technology</i> , 2017, 51, 6279-6287.	4.6	16
8490	Role of the Reducing Agent in the Electroless Deposition of Copper on Functionalized SAMs. <i>Langmuir</i> , 2017, 33, 8663-8670.	1.6	9
8491	Ionic and Neutral Mechanisms for C-H Bond Silylation of Aromatic Heterocycles Catalyzed by Potassium <i>tert</i> -Butoxide. <i>Journal of the American Chemical Society</i> , 2017, 139, 6880-6887.	6.6	111
8492	A theoretical study of the light-induced cross-linking reaction of 5-fluoro-4-thiouridine with thymine. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13524-13533.	1.3	6
8493	A theoretical study of low-lying singlet and triplet excited states of quinazoline, quinoxaline and phthalazine: insight into triplet formation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13828-13837.	1.3	9
8494	Organoboron copolymers containing thienothiophene and selenophenothiophene analogues: optical, electrochemical and fluoride sensing properties. <i>RSC Advances</i> , 2017, 7, 23197-23207.	1.7	12
8495	Dichtefunktionaltheorie: noch nicht ganz die richtige Antwort aus den richtigen Gründen. <i>Angewandte Chemie</i> , 2017, 129, 5482-5484.	1.6	6
8496	Ligand-based studies on cis-stilbene derivatives as cyclo-oxygenase inhibitors. <i>Medicinal Chemistry Research</i> , 2017, 26, 1801-1811.	1.1	2
8497	Cyclohelminthol X, a Hexa-Substituted Spirocyclopropane from <i>Helminthosporium velutinum</i> yone96: Structural Elucidation, Electronic Circular Dichroism Analysis, and Biological Properties. <i>Journal of Organic Chemistry</i> , 2017, 82, 5574-5582.	1.7	28

#	ARTICLE	IF	CITATIONS
8498	Clathrate Structure Determination by Combining Crystal Structure Prediction with Computational and Experimental ¹²⁹ Xe NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2017, 23, 5258-5269.	1.7	18
8499	5-(Hetero)aryl-Substituted 9-Hydroxyphenalenones: Synthesis and Electronic Properties of Multifunctional Donor-Acceptor Conjugates. <i>Chemistry - A European Journal</i> , 2017, 23, 10551-10558.	1.7	4
8500	Accurate prediction of emission energies with TD-DFT methods for platinum and iridium OLED materials. <i>Journal of Molecular Modeling</i> , 2017, 23, 174.	0.8	9
8501	Computational investigation and comparison of hydrogen storage properties of B ₂₄ N ₂₄ and Al ₂₄ N ₂₄ nanocages. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 14166-14180.	3.8	7
8502	Borospherene nanostructure as CO and NO sensor – A first-principles study. <i>Vacuum</i> , 2017, 142, 13-20.	1.6	46
8503	CO ₂ adsorption on different organo-modified SBA-15 silicas: a multidisciplinary study on the effects of basic surface groups. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 14114-14128.	1.3	22
8504	Balance between Metal and Ligand Reduction in Diiminepyridine Complexes of Ti. <i>Organometallics</i> , 2017, 36, 3189-3198.	1.1	14
8505	Theoretical investigation of high-efficiency organic electroluminescent material: HLCT state and hot exciton process. <i>RSC Advances</i> , 2017, 7, 19576-19583.	1.7	48
8506	2 <i>H</i> -Dinaphthopentacene: A Polycyclic Aromatic Hydrocarbon Core for Metal-Free Organic Sensitizers in Efficient Dye-Sensitized Solar Cells. <i>Advanced Science</i> , 2017, 4, 1700099.	5.6	32
8507	Effect of Donors on Photophysical, Electrochemical and Photovoltaic Properties of Benzimidazole-Branched Dyes. <i>ChemistrySelect</i> , 2017, 2, 2807-2814.	0.7	4
8508	NLOphoric 3,6-di(substituted quinoxalin) Carbazoles – Synthesis, Photophysical Properties and DFT Studies. <i>Journal of Fluorescence</i> , 2017, 27, 1531-1540.	1.3	6
8509	New complexes of Cu(II) with dipicolinate and pyridyl-based ligands: An experimental and DFT approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 183, 45-52.	2.0	1
8510	Noble Gas Encapsulated Endohedral Zintl Ions Ng@Pb ₁₂ ²⁺ and Ng@Sn ₁₂ ²⁺ (Ng = He, Ne, Ar, and Kr): A Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11932-11949.	1.5	16
8511	Reduction and oxidation of Au adatoms on the CeO ₂ (111) surface – DFT+U versus hybrid functionals. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12546-12558.	1.3	12
8512	<i>O</i> -Acetyl Side-Chains in Monosaccharides: Redundant NMR Spin-Couplings and Statistical Models for Acetate Ester Conformational Analysis. <i>Journal of Physical Chemistry B</i> , 2017, 121, 66-77.	1.2	25
8513	Syntheses, Structural Characterization, Reactivity, and Theoretical Studies on Some Heteroligand Oxoperoxotungstate(VI). <i>Journal of the Chinese Chemical Society</i> , 2017, 64, 43-54.	0.8	5
8514	The Fractional Occupation Number Weighted Density as a Versatile Analysis Tool for Molecules with a Complicated Electronic Structure. <i>Chemistry - A European Journal</i> , 2017, 23, 6150-6164.	1.7	102
8515	Elucidation of complexation of tetra and hexavalent actinides towards an amide ligand in polar and non-polar diluents: Combined experimental and theoretical approach. <i>Polyhedron</i> , 2017, 123, 234-242.	1.0	4

#	ARTICLE	IF	CITATIONS
8516	The effects of fluorine substitution on the chemical properties and inhibitory capacity of Donepezil anti-Alzheimer drug; density functional theory and molecular docking calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 71, 124-134.	1.3	10
8517	Theoretical investigation of triazine based a star shape pyrrole monomer. <i>Journal of Macromolecular Science - Pure and Applied Chemistry</i> , 2017, 54, 16-23.	1.2	5
8518	Inhibition activities of catechol diether based non-nucleoside inhibitors against the HIV reverse transcriptase variants: Insights from molecular docking and ONIOM calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 294-305.	1.3	11
8519	Atom- and Ion-Centered Icosahedral Shaped Subnanometer-Sized Clusters of Molecular Hydrogen. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15036-15048.	1.5	7
8520	Mechanistic Studies on Pd(MPAA)-Catalyzed Enantioselective C-H Activation Reactions. Springer Theses, 2017, , 83-110.	0.0	0
8521	Radical Reactions Affecting Polar Groups in Threonine Peptide Ions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6557-6569.	1.2	9
8522	Prediction of neutral noble gas compounds LiNgF (Ng = Kr, Xe and Rn). <i>Computational and Theoretical Chemistry</i> , 2017, 1113, 8-13.	1.1	3
8523	Regular and red-shifted fluorescence of the donor-acceptor compound 5-(1H-pyrrole-1-yl)thiophenecarbonitrile (TCN) is efficiently quenched by internal modes of thiophene. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13951-13959.	1.3	3
8524	Mechanistic insights into the light-driven hydrogen evolution reaction from formic acid mediated by an iridium photocatalyst. <i>Catalysis Science and Technology</i> , 2017, 7, 2763-2771.	2.1	7
8525	A theoretical study on the photodissociation mechanism of acetyl fluoride (CH ₃ C(O)F) involving S ₀ , S ₁ , and T ₁ states. <i>Chemical Physics</i> , 2017, 491, 95-101.	0.9	2
8526	Experimental and theoretical investigations on Pd(II) host-guest compound: Deciphering the structural and electronic features of a potential bioactive complex. <i>Journal of Molecular Structure</i> , 2017, 1145, 170-183.	1.8	18
8527	Measurement of reaction rate constants using RCM: A case study of decomposition of dimethyl carbonate to dimethyl ether. <i>Combustion and Flame</i> , 2017, 183, 30-38.	2.8	21
8528	Lithium enhanced second hyperpolarizability of inverse sandwich compounds (M-C ₄ X ₄ -M; X = H, Li) of beryllium, magnesium and calcium. <i>Computational and Theoretical Chemistry</i> , 2017, 1112, 46-51.	1.1	1
8529	TD-DFT Investigation of 2,5-Bis(2-benzothiazolyl)hydroquinone and 2,5-Bis(benzo[d]thiazol-2-yl)-4-methoxyphenol. <i>Journal of Solution Chemistry</i> , 2017, 46, 1005-1023.	0.6	4
8530	Insights on the Reactivity of Terminal Phosphanido Metal Complexes toward Activated Alkynes from Theoretical Computations. <i>Inorganic Chemistry</i> , 2017, 56, 6652-6661.	1.9	2
8531	Comparative study of an osazone based ligand and its palladium(II) complex with human serum albumin: A spectroscopic, thermodynamic and molecular docking approach. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2017, 173, 1-11.	1.7	7
8532	Computational investigation on the large energy gap between the triplet excited-states in acenes. <i>RSC Advances</i> , 2017, 7, 26697-26703.	1.7	26
8533	Synthesis of Benzodihydrofurans by Asymmetric C-H Insertion Reactions of Donor/Donor Rhodium Carbenes. <i>Chemistry - A European Journal</i> , 2017, 23, 11843-11855.	1.7	43

#	ARTICLE	IF	CITATIONS
8534	Study of Alcohol and Aldehydes Interaction on the Surface of Silicane Nanosheet: Application of Density Functional Theory. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2017, 27, 1307-1316.	1.9	16
8535	Exciton coupling between enones: Quassinoids revisited. <i>Chirality</i> , 2017, 29, 476-485.	1.3	16
8536	Molecular simulation of CO ₂ /CH ₄ adsorption in brown coal: Effect of oxygen-, nitrogen-, and sulfur-containing functional groups. <i>Applied Surface Science</i> , 2017, 423, 33-42.	3.1	99
8537	Charge Transfer Properties of Triarylamine Integrated Dimolybdenum Dyads. <i>Inorganic Chemistry</i> , 2017, 56, 7470-7481.	1.9	14
8538	A Strategy for the Synthesis of 1,2-Dichlorotetrafluorocyclobutene from Hexachlorobutadiene and Its Reaction Pathway. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 7623-7630.	1.8	9
8539	Dissecting the accountability of parameterized and parameter-free single-hybrid and double-hybrid functionals for photophysical properties of TADF-based OLEDs. <i>Journal of Chemical Physics</i> , 2017, 146, 234304.	1.2	17
8540	Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. <i>Molecular Physics</i> , 2017, 115, 2315-2372.	0.8	1,401
8541	Mechanistic Insights on the Reduction of CO ₂ to Silylformates Catalyzed by Ir ^{III} Species. <i>Chemistry - A European Journal</i> , 2017, 23, 11898-11907.	1.7	30
8542	How seaweeds release the excess energy from sunlight to surrounding sea water. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15745-15753.	1.3	17
8543	Ultrafast Excited-State Deactivation Dynamics of Cyclotrisazobenzene: A Novel Type of UV-A Absorber. <i>ChemPhysChem</i> , 2017, 18, 2137-2141.	1.0	17
8544	Exploring the impacts of the vinylogous anomeric effect on the synchronous early and late transition states of the hydrogen molecule elimination reactions of cis-3,6-dihalocyclohexa-1,4-dienes. <i>Structural Chemistry</i> , 2017, 28, 1803-1814.	1.0	16
8545	Protonation-Induced Sign Inversion of the Cotton Effects of Pyridinophanes. A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 977-985.	1.1	10
8546	QTAIM and Stress Tensor Characterization of Intramolecular Interactions Along Dynamics Trajectories of a Light-Driven Rotary Molecular Motor. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4778-4792.	1.1	17
8547	Roles of the Active Site Zn(II) and Residues in Substrate Discrimination by Threonyl-tRNA Synthetase: An MD and QM/MM Investigation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6163-6174.	1.2	8
8548	Computational insights into substrate binding and catalytic mechanism of the glutaminase domain of glucosamine-6-phosphate synthase (GlmS). <i>RSC Advances</i> , 2017, 7, 29626-29638.	1.7	5
8549	Molecular design and theoretical investigation of new metal-free heteroaromatic dyes with D-π-A architecture as photosensitizers for DSSC application. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 345, 63-73.	2.0	49
8550	A DFT study on the mechanism of NO decomposition catalyzed by short-distance Cu(I) pairs in Cu-ZSM-5. <i>Molecular Catalysis</i> , 2017, 434, 96-105.	1.0	13
8551	New Class of Organic Hole-Transporting Materials Based on Xanthene Derivatives for Organic Electronic Applications. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12999-13007.	1.5	13

#	ARTICLE	IF	CITATIONS
8552	Covalent Co–O–V and Sb–N Bonds Enable Polyoxovanadate Charge Control. <i>Inorganic Chemistry</i> , 2017, 56, 7120-7126.	1.9	15
8553	Linker Effects in Porphyrin Polymeric Donor Materials for Photovoltaic Devices. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12018-12024.	1.5	6
8554	Characterization of Protonated Model Disaccharides from Tandem Mass Spectrometry and Chemical Dynamics Simulations. <i>ChemPhysChem</i> , 2017, 18, 2812-2823.	1.0	22
8555	DFT study on abstraction reaction mechanism of OH radical with 2-methoxyphenol. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3713.	0.9	15
8556	Novel enantioselective fluorescent sensors for tartrate anion based on acridinezswsxa. <i>Luminescence</i> , 2017, 32, 1313-1318.	1.5	10
8557	Metal-Dependent Strengthening and Weakening of M–H and M–C Bonds by an Oxo Ligand: Thermal Gas-Phase Activation of Methane by [OMH] ⁺ and [MH] ⁺ (M=Mo, Ti). <i>Chemistry - A European Journal</i> , 2017, 23, 12346-12352.	1.7	7
8558	Stable 5,5-Substituted 2,2-Bipyrroles: Building Blocks for Macrocyclic and Materials Chemistry. <i>Journal of Organic Chemistry</i> , 2017, 82, 6904-6912.	1.7	7
8559	Structural Distortions and Charge Density Waves in Iodine Chains Encapsulated inside Carbon Nanotubes. <i>Nano Letters</i> , 2017, 17, 3694-3700.	4.5	44
8560	BN-Heterocycles Bearing Two BN Units: Influence of the Linker and the Location of BN Units on Electronic Properties and Photoreactivity. <i>Organometallics</i> , 2017, 36, 2654-2660.	1.1	22
8561	Effect of Point Defects on Optical Properties of Graphene Fluoride: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12855-12862.	1.5	30
8562	Zinc(II) bis(dipyromethene)s crystal solvates with dimethyl sulfoxide Composition, stability and spectral-luminescent properties. <i>Sensors and Actuators B: Chemical</i> , 2017, 251, 858-868.	4.0	15
8563	Role of asymmetric magnetic electrodes in tuning spin selective rectification action of borazine [B ₃ N ₃ H ₆]. <i>Chemical Physics</i> , 2017, 491, 126-135.	0.9	3
8564	Reaction Mechanism of Cu(I)-Mediated Reductive CO ₂ Coupling for the Selective Formation of Oxalate: Cooperative CO ₂ Reduction To Give Mixed-Valence Cu ₂ (CO ₂) ⁺ and Nucleophilic-Like Attack. <i>Inorganic Chemistry</i> , 2017, 56, 6809-6819.	1.9	39
8565	Ferromagnetic Exchange Coupling in a Family of Mn ^{III} Salen-Type Schiff-Base Out-of-Plane Dimers. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12454-12468.	1.5	18
8566	Influence of Extended Conjugation on Photophysical/Electronic Properties and Photoelimination of BN-Heterocycles. <i>Organometallics</i> , 2017, 36, 2677-2684.	1.1	8
8567	Structure and spin state of nonheme Fe ^{IV} O complexes depending on temperature: predictive insights from DFT calculations and experiments. <i>Chemical Science</i> , 2017, 8, 5460-5467.	3.7	25
8568	Switch effect of the nonquantized intrinsic spin Hall conductivity in monolayered monoclinic transition metal dichalcogenides. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 295302.	0.7	1
8569	Studying physisorption processes and molecular friction of cycloparaphenylene molecules on graphene nano-sized flakes: role of π–π and CH–π interactions. <i>Molecular Systems Design and Engineering</i> , 2017, 2, 253-262.	1.7	7

#	ARTICLE	IF	CITATIONS
8570	Dithiafulvenyl-Extended $\langle i \rangle N \langle /i \rangle$ -Heterotriangulenes and Their Interaction with C_{60} : Cooperative Fluorescence. <i>Chemistry - A European Journal</i> , 2017, 23, 12353-12362.	1.7	8
8571	Design of Highly Selective Alkyne Hydrothiolation Rh^{I} -NHC Catalysts: Carbonyl-Triggered Nonoxidative Mechanism. <i>Organometallics</i> , 2017, 36, 2198-2207.	1.1	34
8572	The Origins of Dramatic Differences in Five-Membered vs Six-Membered Chelation of Pd(II) on Efficiency of $C(sp^3)$ -H Bond Activation. <i>Journal of the American Chemical Society</i> , 2017, 139, 8514-8521.	6.6	96
8573	Simple Fully Nonlocal Density Functionals for Electronic Repulsion Energy. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2799-2805.	2.1	30
8574	Synthesis and fluorosolvatochromic properties of 1,7-annulated indoles. <i>New Journal of Chemistry</i> , 2017, 41, 7331-7338.	1.4	5
8575	Can DFT and ab initio methods adequately describe binding energies in strongly interacting $C_6X_6 \cdot C_2X_2$ complexes?. <i>Chemical Physics</i> , 2017, 493, 12-19.	0.9	7
8576	Tuning Near-Infrared Absorbing Donor Materials: A Study of Electronic, Optical, and Charge-Transport Properties of aza-BODIPYs. <i>Chemistry of Materials</i> , 2017, 29, 5525-5536.	3.2	31
8577	Catalytic N_2 Reduction to Silylamines and Thermodynamics of N_2 Binding at Square Planar Fe. <i>Journal of the American Chemical Society</i> , 2017, 139, 9291-9301.	6.6	72
8578	On the feasibility of reactions through the fullerene wall: a theoretical study of $NH_x @ C_{60}$. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17199-17209.	1.3	4
8579	Inside information on xenon adsorption in porous organic cages by NMR. <i>Chemical Science</i> , 2017, 8, 5721-5727.	3.7	37
8580	Electronic Properties of a New All-Inorganic Perovskite $TiPb_3$ Simulated by the First Principles. <i>Nanoscale Research Letters</i> , 2017, 12, 232.	3.1	11
8581	Investigation on terpolymer of ethylene/propylene/1-bromo-1-olefins catalyzed by titanium complexes. <i>Journal of Materials Science</i> , 2017, 52, 5981-5991.	1.7	6
8582	Channeling through Two Stacked Guanine Quartets of One and Two Alkali Cations in the Li^+ , Na^+ , K^+ , and Rb^+ Series. Assessment of the Accuracy of the SIBFA Anisotropic Polarizable Molecular Mechanics Potential. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3997-4014.	1.2	20
8583	Characterization of charge transfer mechanisms in the molecular capacitor \hat{I}^2 -DiCC[Ni(dmit) ₂] using TD-DFT methods. <i>Computational and Theoretical Chemistry</i> , 2017, 1109, 36-41.	1.1	2
8584	The mechanism of the gas-phase elimination kinetics of the \hat{I}^2, \hat{I}^3 -unsaturated aldehyde 2,2-dimethyl-3-butenal: a theoretical study. <i>Molecular Physics</i> , 2017, 115, 1624-1632.	0.8	2
8585	The mechanism of the Ser-(cis)Ser-Lys catalytic triad of peptide amidases. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12343-12354.	1.3	17
8586	Radical cation and dication of a 4H-dithieno[2,3-b:3',2'-e][1,4]-thiazine. <i>Organic Chemistry Frontiers</i> , 2017, 4, 839-846.	2.3	10
8587	Croconato-bridged copper(II) complexes: synthesis, structure and magnetic characterization. <i>New Journal of Chemistry</i> , 2017, 41, 3846-3856.	1.4	5

#	ARTICLE	IF	CITATIONS
8588	Effects of energy correlations and superexchange on charge transport and exciton formation in amorphous molecular semiconductors: An <i>ab initio</i> study. <i>Physical Review B</i> , 2017, 95, .	1.1	33
8589	A theoretical investigation on doping superalkali for triggering considerable nonlinear optical properties of Si ₁₂ C ₁₂ nanostructure. <i>Journal of Computational Chemistry</i> , 2017, 38, 1574-1582.	1.5	43
8590	Effects of the locality of a potential derived from hybrid density functionals on Kohn–Sham orbitals and excited states. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10177-10186.	1.3	14
8591	UNO DMRG CASCI calculations of effective exchange integrals for m-phenylene-bis-methylene spin clusters. <i>Molecular Physics</i> , 2017, 115, 2154-2167.	0.8	2
8592	Quantum Chemical Strain Analysis For Mechanochemical Processes. <i>Accounts of Chemical Research</i> , 2017, 50, 1041-1048.	7.6	35
8593	Excited-State Decay Paths in Tetraphenylethene Derivatives. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2572-2579.	1.1	93
8594	Lattice energetics and thermochemistry of acridine derivatives and substituted acridinium trifluoromethanesulphonates. <i>Journal of Thermal Analysis and Calorimetry</i> , 2017, 129, 1613-1624.	2.0	3
8595	Room temperature phosphorescence lifetime and spectrum tuning of substituted thianthrenes. <i>Dyes and Pigments</i> , 2017, 142, 315-322.	2.0	35
8596	Temperature-Programmed Desorption (TPD) and Density Functional Theory (DFT) Study Comparing the Adsorption of Ethyl Halides on the Si(100) Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 7208-7213.	1.5	3
8597	A Theoretical Study on Methane C–H Bond Activation by Bare [FeO] ^{+0/â€“} . <i>Journal of Physical Chemistry A</i> , 2017, 121, 3501-3514.	1.1	16
8598	Computationally predicted energies and properties of defects in GaN. <i>Npj Computational Materials</i> , 2017, 3, .	3.5	196
8599	A Computational Way To Achieve More Effective Candidates for Photodynamic Therapy. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1089-1100.	2.5	17
8600	Ruthenium PNN(O) Complexes: Cooperative Reactivity and Application as Catalysts for Acceptorless Dehydrogenative Coupling Reactions. <i>Organometallics</i> , 2017, 36, 1541-1549.	1.1	53
8601	Quantum and Statistical Mechanical Simulations for Porous Catalyst Modelling. , 2017, , 253-288.		2
8602	White Light Emitting Polymers Possessing Thienothiophene and Boron Units. <i>ChemistrySelect</i> , 2017, 2, 2889-2894.	0.7	14
8603	Strongly Circularly Polarized Emission from Water-Soluble Eu(III)- and Tb(III)-Based Complexes: A Structural and Spectroscopic Study. <i>Inorganic Chemistry</i> , 2017, 56, 4413-4421.	1.9	60
8604	Mechanism of Cytochrome P450 17A1-Catalyzed Hydroxylase and Lyase Reactions. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1123-1133.	2.5	24
8606	Theoretical study of HNCO formation from atomic nitrogen and carbon monoxide in the presence of water. <i>Chemical Physics</i> , 2017, 488-489, 28-35.	0.9	0

#	ARTICLE	IF	CITATIONS
8607	Synthetic and Structural Studies on Linear and Macrocyclic Pd- and Pt-Bridged Butterfly Fe/S Cluster Complexes. <i>Organometallics</i> , 2017, 36, 1419-1429.	1.1	5
8608	Primary hydration and proton transfer of electrolyte acids: An ab initio study. <i>Solid State Ionics</i> , 2017, 306, 2-12.	1.3	16
8609	Degradation of Hole Transport Materials via Exciton-Driven Cyclization. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 13369-13379.	4.0	14
8610	Electronic Structure Studies on the Whole Keplerate Family: Predicting New Members. <i>Chemistry - A European Journal</i> , 2017, 23, 5338-5344.	1.7	4
8611	Aggregation induced emissive and NLOphoric coumarin thiazole hybrid dyes: Synthesis, photophysics and TD-DFT studies. <i>Journal of Luminescence</i> , 2017, 188, 38-53.	1.5	13
8612	Testing Exact Upper Bounds to Exact Exchange. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1980-1988.	2.3	3
8614	Silver Deposition onto Modified Silicon Substrates. <i>Journal of Physical Chemistry C</i> , 2017, 121, 7240-7247.	1.5	7
8615	Can there be a multi-bond between noble gas and metal? A theoretical study of F ₂ XeMoF ₂ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 9545-9550.	1.3	8
8616	Metal-free catalytic conversion of CO ₂ and glycerol to glycerol carbonate. <i>Green Chemistry</i> , 2017, 19, 1775-1781.	4.6	64
8617	Z2Pack: Numerical implementation of hybrid Wannier centers for identifying topological materials. <i>Physical Review B</i> , 2017, 95, .	1.1	322
8618	The Biophysical Probes 2-fluorohistidine and 4-fluorohistidine: Spectroscopic Signatures and Molecular Properties. <i>Scientific Reports</i> , 2017, 7, 42651.	1.6	5
8619	N ₂ O Formation via Reductive Disproportionation of NO by Mononuclear Copper Complexes: A Mechanistic DFT Study. <i>Inorganic Chemistry</i> , 2017, 56, 3820-3833.	1.9	25
8620	Effect of Substituent on the Mechanism and Chemoselectivity of the Gold(I)-Catalyzed Propargyl Ester Tandem Cyclization. <i>Organometallics</i> , 2017, 36, 1164-1172.	1.1	22
8621	Origin of non-conservative circular dichroism of the CP29 antenna complex of photosystem II. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7524-7536.	1.3	22
8622	The cyclopropanation of [60]fullerobenzofurans via electrocatalysis. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 3248-3254.	1.5	12
8623	Molecular simulation and experiments of water adsorption in a high surface area activated carbon: Hysteresis, scanning curves and spatial organization of water clusters. <i>Carbon</i> , 2017, 118, 127-138.	5.4	49
8624	Conformational Populations of ¹³ C-(1 ^H)-Glycosidic Linkages Using Redundant NMR ¹³ C- ¹ H-Couplings and Circular Statistics. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3042-3058.	1.2	39
8625	Role of exact exchange in thermally-assisted-occupation density functional theory: A proposal of new hybrid schemes. <i>Journal of Chemical Physics</i> , 2017, 146, 044102.	1.2	38

#	ARTICLE	IF	CITATIONS
8626	Density functional modelling studies of chloride-substituted Schiff bases as corrosion inhibitors: Optimized geometries, atomic charges, solvent and non-linear optical effects. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2017, 53, 159-176.	0.3	3
8627	Mechanism and Kinetics of the Reaction of Nitrosamines with OH Radical: A Theoretical Study. <i>International Journal of Chemical Kinetics</i> , 2017, 49, 339-353.	1.0	14
8628	Towards designing polymers for photovoltaic applications: A DFT and experimental study of polyazomethines with various chemical structures. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 181, 208-217.	2.0	12
8629	Cavity Ringdown Spectrum of 2-Cyclohexen-1-one in the CO/Alkenyl CC Stretch Region of the S1(n, Tj) ETQq1 1 0.784314 rgBT / Over	1.1	2
8630	Ferrocene-based diradicals of imino nitroxide, nitronyl nitroxide and verdazyl, and their cations are possible SMM: A quantum chemical study. <i>Chemical Physics Letters</i> , 2017, 676, 70-76.	1.2	9
8631	Benchmark Study of Density Functional Theory for Neutral Gold Clusters, Au _n ($n = 2\text{--}8$). <i>Journal of Physical Chemistry A</i> , 2017, 121, 2410-2419.	1.1	34
8632	Large, weakly basic bis(carboranyl)phosphines: an experimental and computational study. <i>Dalton Transactions</i> , 2017, 46, 5218-5228.	1.6	18
8633	Reduction of [Cp*Sb] ₄ with Subvalent Main-Group Metal Reductants: Syntheses and Structures of [(L ¹ Mg) ₄ (Sb ₄)] and [(L ² Ga) ₂ (Sb ₄)] Containing Edge-Missing Sb ₄ Units. <i>Chemistry - A European Journal</i> , 2017, 23, 2461-2468.	1.7	36
8634	CO oxidation by the atomic oxygen on silver clusters: structurally dependent mechanisms generating free or chemically bonded CO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 196-203.	1.3	22
8635	Formation and Unimolecular Dehydrogenation of Gaseous Alkaline-earth Metal Amidoboranes M(NH ₂ BH ₃) ₂ (M = Be - Ba): Comparative Computational Study. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2017, 643, 209-213.	0.6	2
8636	Effect of doping and chemical ordering on the optoelectronic properties of complex oxides: Fe ₂ O ₃ ∕V ₂ O ₃ solid solutions and hetero-structures. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1097-1107.	1.3	4
8637	Correlating excited state and charge carrier dynamics with photovoltaic parameters of perylene dye sensitized solar cells: influences of an alkylated carbazole ancillary electron-donor. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2549-2556.	1.3	8
8638	Multi-substituted deep-blue emitting carbazoles: a comparative study on photophysical and electroluminescence characteristics. <i>Journal of Materials Chemistry C</i> , 2017, 5, 709-726.	2.7	47
8639	Emerging New Pseudobinary and Ternary Halides as Scintillators for Radiation Detection. <i>IEEE Transactions on Nuclear Science</i> , 2017, 64, 1817-1824.	1.2	9
8640	Stereochemical and electronic interaction studies of 4- <i>substituted</i> 2-(phenylselanyl)-2-(ethylsulfinyl)-acetophenones. <i>Journal of Molecular Structure</i> , 2017, 1133, 49-65.	1.8	3
8641	Cu and Ag complex formation with the hydrophilic phosphine 1,3,5-triaza-7-phosphadamantane in different ionic media. How to estimate the effect of a complexing medium. <i>Dalton Transactions</i> , 2017, 46, 1455-1466.	1.6	29
8642	Evaluation of density functionals for elementary steps of selective oxidation reactions. <i>Computational and Theoretical Chemistry</i> , 2017, 1101, 36-45.	1.1	11
8643	Spectral Features and Excited-State Transformations of Hydroxy Derivatives of 4-Dimethylaminoflavone in PVA Films and on Plasmonic Platforms. <i>Journal of Physical Chemistry C</i> , 2017, 121, 636-648.	1.5	6

#	ARTICLE	IF	CITATIONS
8644	The mechanism determination of trimer and tetramer HCN for adenine formation in the gas phase of interstellar space. <i>Computational and Theoretical Chemistry</i> , 2017, 1101, 68-73.	1.1	7
8645	Thermochemical and Kinetics of CH ₃ SH + H Reactions: The Sensitivity of Coupling the Low and High-Level Methodologies. <i>Journal of Physical Chemistry A</i> , 2017, 121, 419-428.	1.1	10
8646	Stationary Conditions of the Electron Density Along the Reaction Path: Connection with Conceptual DFT and Information Theory. <i>Journal of Physical Chemistry A</i> , 2017, 121, 648-660.	1.1	10
8647	Approximate Force Constants from Uncoupled Self-Consistent Field Perturbation Theory Using Nonhybrid Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2017, 121, 348-356.	1.1	1
8648	Investigating the Interaction of Water Vapour with Aminopropyl Groups on the Surface of Mesoporous Silica Nanoparticles. <i>ChemPhysChem</i> , 2017, 18, 839-849.	1.0	21
8649	Formulation of water to ethanol ratio as extraction solvents of <i>Ixora coccinea</i> and <i>Bougainvillea glabra</i> and their effect on dye aggregation in relation to DSSC performance. <i>Ionics</i> , 2017, 23, 485-495.	1.2	11
8650	Rapid Method Development in Hydrophilic Interaction Liquid Chromatography for Pharmaceutical Analysis Using a Combination of Quantitative Structure-Retention Relationships and Design of Experiments. <i>Analytical Chemistry</i> , 2017, 89, 1870-1878.	3.2	41
8651	Total Facial Discrimination of 1,3-Dipolar Cycloadditions in a <i>d</i> -Erythrose 1,3-Dioxane Template: Computational Studies of a Concerted Mechanism. <i>Journal of Organic Chemistry</i> , 2017, 82, 982-991.	1.7	6
8652	Effects of different electron donating groups on dye regeneration and aggregation in phenothiazine-based dye-sensitized solar cells. <i>Organic Electronics</i> , 2017, 42, 234-243.	1.4	25
8653	The Solvation Structure of Lithium Ions in an Ether Based Electrolyte Solution from First-Principles Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2017, 121, 180-188.	1.2	41
8654	Excited-State and Charge Carrier Dynamics in a High-Photovoltage and Thermostable Dye-Sensitized Solar Cell. <i>ACS Photonics</i> , 2017, 4, 165-173.	3.2	17
8655	Doped fullerene as a metal-free electrocatalyst for oxygen reduction reaction: A first-principles study. <i>Carbon</i> , 2017, 114, 393-401.	5.4	82
8656	Machine Learning Methods to Predict Density Functional Theory B3LYP Energies of HOMO and LUMO Orbitals. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 11-21.	2.5	129
8657	Diaquabis(ethylenediamine)copper(II) vs. monoaquabis(ethylenediamine)copper(II): Synthesis, characterization, single crystal X-ray structure determination, theoretical calculations and antimicrobial activities of [Cu(en) ₂ (H ₂ O) ₂](2-phenoxybenzoate) ₂ ·H ₂ O and [Cu(en) ₂ (H ₂ O)](diphenylacetate) ₂ ·3H ₂ O. <i>Polyhedron</i> , 2017, 123, 430-440.	1.0	14
8658	A structure-property interplay between the width and height of cages and the static third order nonlinear optical responses for fullerenes: applying gamma density analysis. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2322-2331.	1.3	20
8659	Three-state conical intersection optimization methods: development and implementation at QM/MM level. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	26
8660	Accurate Dissociation of Chemical Bonds Using DFT-in-DFT Embedding Theory with External Orbital Orthogonality. <i>Journal of Physical Chemistry A</i> , 2017, 121, 256-264.	1.1	24
8661	Studies on anticorrosive action of synthesized indolines on mild steel in 15% HCl solution. <i>Journal of Adhesion Science and Technology</i> , 2017, 31, 1524-1544.	1.4	16

#	ARTICLE	IF	CITATIONS
8662	Optical properties and component composition of layers of cyanine dyes on dielectric supports: influence of asymmetry of the molecular electron density distribution. <i>Optical and Quantum Electronics</i> , 2017, 49, 1.	1.5	6
8663	Cyclopentadienone iron complexes as efficient and selective catalysts for the electroreduction of CO ₂ to CO. <i>Catalysis Science and Technology</i> , 2017, 7, 459-465.	2.1	41
8664	Divergent reactivity of a new dinuclear xantheno-bridged bis(iminopyridine) di-nickel complex with alkynes. <i>Dalton Transactions</i> , 2017, 46, 5605-5616.	1.6	29
8665	Judicious engineering of a metal-free perylene dye for high-efficiency dye sensitized solar cells: the control of excited state and charge carrier dynamics. <i>Journal of Materials Chemistry A</i> , 2017, 5, 3514-3522.	5.2	18
8666	Oxidative Coupling of Imino, Amide Platinum(II) Complexes Yields Highly Conjugated Blue Dimers. <i>Organometallics</i> , 2017, 36, 384-390.	1.1	15
8667	Photochromic Mechanism of a Bridged Diarylethene: Combined Electronic Structure Calculations and Nonadiabatic Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 793-802.	1.1	7
8668	p-Doping of polystyrene polymers with attached functional side-groups from solution. <i>Journal of Materials Chemistry C</i> , 2017, 5, 770-776.	2.7	13
8669	Theoretical Investigation on the ClBcat-Promoted Synthesis of Heterocyclic Boronic Esters. <i>Asian Journal of Organic Chemistry</i> , 2017, 6, 282-289.	1.3	9
8670	Initial stage of the degradation of three common neonicotinoids: theoretical prediction of charge transfer sites. <i>New Journal of Chemistry</i> , 2017, 41, 965-974.	1.4	8
8671	Complex beryllium amidoboranes: Structures, stability, and evaluation of their potential as hydrogen storage materials. <i>Journal of Computational Chemistry</i> , 2017, 38, 401-405.	1.5	5
8672	<i>mer</i> , <i>fac</i> , and Bidentate Coordination of an Alkyl-POP Ligand in the Chemistry of Nonclassical Osmium Hydrides. <i>Inorganic Chemistry</i> , 2017, 56, 676-683.	1.9	29
8673	The Variediene-Forming Carbocation Cyclization/Rearrangement Cascade. <i>Australian Journal of Chemistry</i> , 2017, 70, 362.	0.5	18
8674	Iodate in calcite and vaterite: Insights from synchrotron X-ray absorption spectroscopy and first-principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2017, 198, 218-228.	1.6	56
8675	Activation of the dimers and tetramers of metal amidinate atomic layer deposition precursors upon adsorption on silicon oxide surfaces. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2017, 35, .	0.9	12
8676	Intramolecular single H bonding vs bifurcation in tuning the conformation of 2,2'-dihydroxybenzophenone and its derivatives: a DFT insight. <i>Structural Chemistry</i> , 2017, 28, 925-943.	1.0	5
8677	Prediction of retention in hydrophilic interaction liquid chromatography using solute molecular descriptors based on chemical structures. <i>Journal of Chromatography A</i> , 2017, 1486, 59-67.	1.8	47
8678	An EOM-CCSD-PCM Benchmark for Electronic Excitation Energies of Solvated Molecules. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 117-124.	2.3	22
8679	Ab Initio Calculations on some Antiepileptic Drugs such as Phenytoin, Phenobarbital, Ethosuximide and Carbamazepine. <i>Structural Chemistry</i> , 2017, 28, 957-964.	1.0	34

#	ARTICLE	IF	CITATIONS
8680	Four- and Five-Component Syntheses and Photophysical Properties of Emission Solvatochromic 3-Aminovinylquinoxalines. <i>Journal of Organic Chemistry</i> , 2017, 82, 567-578.	1.7	32
8681	A Rapid and Facile Detection for Specific Small-Sized Amino Acids Based on Target-Triggered Destruction of Metal Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 236-243.	4.0	44
8682	NO ₂ adsorption behaviour on germanene nanosheet – A first-principles investigation. <i>Superlattices and Microstructures</i> , 2017, 101, 160-171.	1.4	50
8683	Synthesis, structural characterization and computational study of a novel amino chalcone: a potential nonlinear optical material. <i>New Journal of Chemistry</i> , 2017, 41, 1744-1754.	1.4	61
8684	A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32184-32215.	1.3	1,230
8685	<i>Ab initio</i> simulations of water splitting on hematite. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 463002.	0.7	17
8687	TADF Material Design: Photophysical Background and Case Studies Focusing on Cu ^I and Ag ^I Complexes. <i>ChemPhysChem</i> , 2017, 18, 3508-3535.	1.0	190
8688	Molecular Origin of the Anisotropic Dye Orientation in Emissive Layers of Organic Light Emitting Diodes. <i>Chemistry of Materials</i> , 2017, 29, 9528-9535.	3.2	39
8689	Novel thienoisindigo-based dyes for near-infrared organic photovoltaics - A combination of theoretical and experimental study. <i>Organic Electronics</i> , 2017, 51, 410-421.	1.4	5
8690	Relevance of the DFT method to study expanded porphyrins with different topologies. <i>Journal of Computational Chemistry</i> , 2017, 38, 2819-2828.	1.5	64
8691	Role of Exact Exchange and Relativistic Approximations in Calculating ¹⁹ F Magnetic Shielding in Solids Using a Cluster Ansatz. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4741-4752.	2.3	20
8692	Intermolecular magnetic interactions in stacked DNA base pairs. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27817-27827.	1.3	5
8693	Electronic Properties of Bulk and Monolayer TMDs: Theoretical Study Within DFT Framework (GV) ² e Tj ETQq0 0,0 rgBT /Overlock 10 0.85 277	0.85	277
8694	The ionic versus metallic nature of 2D electriles: a density-functional description. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27343-27352.	1.3	16
8695	Embedding for bulk systems using localized atomic orbitals. <i>Journal of Chemical Physics</i> , 2017, 147, 034110.	1.2	17
8696	Development of a TDDFT-Based Protocol with Local Hybrid Functionals for the Screening of Potential Singlet Fission Chromophores. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4984-4996.	2.3	57
8697	The optoelectronic properties of organic materials based on triphenylamine that are relevant to organic solar photovoltaic cells. <i>New Journal of Chemistry</i> , 2017, 41, 13336-13346.	1.4	38
8698	HOMO inversion as a strategy for improving the light-absorption properties of Fe(ⁱⁱ) chromophores. <i>Chemical Science</i> , 2017, 8, 8115-8126.	3.7	52

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8699	Comparative density functional theoryâ€“density functional tight binding study of fullerene derivatives: effects due to fullerene size, addends, and crystallinity on band structure, charge transport and optical properties. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28330-28343.	1.3	23
8700	Experimental Charge-Density Study of the Intra- and Intermolecular Bonding in TKX-50. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8962-8972.	1.1	16
8701	Crystal structures and magnetic properties of two series of phenoxo- <i>O</i> bridged dinuclear Ln ₂ (Ln = Gd, Tb, Dy) complexes. <i>Dalton Transactions</i> , 2017, 46, 16294-16305.	1.6	34
8702	Novel HDAC8 inhibitors: A multi-computational approach. <i>SAR and QSAR in Environmental Research</i> , 2017, 28, 707-733.	1.0	7
8703	Tracking the Chemical Transformations at the Brønsted Acid Site upon Water-Induced Deprotonation in a Zeolite Pore. <i>Chemistry of Materials</i> , 2017, 29, 9030-9042.	3.2	71
8704	Rational In Silico Design of an Organic Semiconductor with Improved Electron Mobility. <i>Advanced Materials</i> , 2017, 29, 1703505.	11.1	27
8705	First-principles calculation of intrinsic defect chemistry and self-doping in PbTe. <i>Npj Computational Materials</i> , 2017, 3, .	3.5	62
8706	Cleaving Off Uranyl Oxygens through Chelation: A Mechanistic Study in the Gas Phase. <i>Inorganic Chemistry</i> , 2017, 56, 12930-12937.	1.9	23
8707	Improving the Efficiency of Beyond-RPA Methods within the Dielectric Matrix Formulation: Algorithms and Applications to the A24 and S22 Test Sets. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5432-5442.	2.3	16
8708	Synthesis of aza-pseudopeptides and the evaluation of their inhibiting efficacy of mild steel corrosion in 1.0 M HCl. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2017, 53, 928-936.	0.3	5
8709	Structural and Vibrational Properties of Iodopentafluorobenzene: A Combined Raman and Infrared Spectral and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7917-7924.	1.1	3
8710	Synthesis and Reactivities of Polyhydrido Osmium Arylsilyl Complexes Prepared from OsH ₃ Cl(PPh ₃) ₃ . <i>Organometallics</i> , 2017, 36, 3729-3738.	1.1	6
8711	Reduction of Diphenylacetylene Mediated by Rare-Earth Ferrocene Diamide Complexes. <i>Organometallics</i> , 2017, 36, 4643-4648.	1.1	20
8712	Rigid fused Ñ-spacers in D-Ñ type molecules for dye-sensitized solar cells: a computational investigation. <i>Journal of Materials Chemistry C</i> , 2017, 5, 11454-11465.	2.7	56
8713	Excited-state absorption in tetrapyrrolyl porphyrins: comparing real-time and quadratic-response time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27452-27462.	1.3	32
8714	Mechanistic insights into the Î³-elimination reaction of l-methionine catalyzed by methionine Î³-lyase (MGL). <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	6
8715	Keto-enol heterocycles as new compounds of corrosion inhibitors for carbon steel in 1 M HCl: Weight loss, electrochemical and quantum chemical investigation. <i>Journal of Molecular Liquids</i> , 2017, 248, 340-349.	2.3	108
8716	Triaryl-Boron Functionalized Dinuclear Platinum Complexes Linked by Photoisomerizable Bpe Ligand: Luminescence and Isomerism. <i>Inorganic Chemistry</i> , 2017, 56, 12783-12794.	1.9	11

#	ARTICLE	IF	CITATIONS
8717	Direct Evidence for Neutral <i>N</i> -Pyrazolyl Radicals: Paddlewheel Dibismuthanes Bearing Pyrazolato Ligands with Very Short Bi–Bi Single Bonds. <i>Inorganic Chemistry</i> , 2017, 56, 12678-12681.	1.9	19
8718	Picosecond sulfur K-edge X-ray absorption spectroscopy with applications to excited state proton transfer. <i>Structural Dynamics</i> , 2017, 4, 044021.	0.9	15
8719	Hybrid-DFT+ <i>V</i> method for band structure calculation of semiconducting transition metal compounds: the case of cerium dioxide. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 454002.	0.7	5
8720	MD/QC Simulation of the Structure and Spectroscopic Properties of $\hat{\pm}$ -NPD-BAlq Exciplexes at an $\hat{\pm}$ -NPD/BAlq Interface in OLEDs. <i>ChemistrySelect</i> , 2017, 2, 9495-9500.	0.7	3
8721	Selective Hybridization of a Terpyridine-Based Molecule with a Noble Metal. <i>Journal of Physical Chemistry C</i> , 2017, 121, 23574-23581.	1.5	4
8722	Interpolative Separable Density Fitting Decomposition for Accelerating Hybrid Density Functional Calculations with Applications to Defects in Silicon. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5420-5431.	2.3	53
8723	Experimental and Computational Gas Phase Acidities of Conjugate Acids of Triazolylidene Carbenes: Rationalizing Subtle Electronic Effects. <i>Journal of the American Chemical Society</i> , 2017, 139, 14917-14930.	6.6	33
8724	Intramolecular London Dispersion Interaction Effects on Gas-Phase and Solid-State Structures of Diamondoid Dimers. <i>Journal of the American Chemical Society</i> , 2017, 139, 16696-16707.	6.6	62
8725	Effect of donor to acceptor ratio on electrochemical and spectroscopic properties of oligoalkylthiophene 1,3,4-oxadiazole derivatives. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30261-30276.	1.3	20
8726	Two-Dimensional Arrangements of Bis(haloethynyl)benzenes Combining Halogen and Hydrogen Interactions. <i>Crystal Growth and Design</i> , 2017, 17, 6212-6223.	1.4	16
8727	Further insight into the electrocatalytic water oxidation by macrocyclic nickel(<i>ii</i>) complexes: the influence of steric effect on catalytic activity. <i>Catalysis Science and Technology</i> , 2017, 7, 5585-5593.	2.1	35
8728	Interrogating the Becke+ TM 05 density functional for non-locality information. <i>Journal of Chemical Physics</i> , 2017, 147, 154103.	1.2	15
8729	Diffusion of Fission Gas in Uranium Dioxide: A First-Principles Study. , 2017, , .		0
8730	Luminophore from forgotten dye: di(Alkylthiophene) derivative of benzo[<i>h</i>]benz[5,6]acridino[2,1,9,8- <i>klmna</i>]acridine. <i>Synthetic Metals</i> , 2017, 232, 117-122.	2.1	5
8731	On the Origin of the 3.3 $\hat{1}$ / ₄ μ m Unidentified Infrared Emission Feature. <i>Astrophysical Journal</i> , 2017, 845, 123.	1.6	11
8732	Theoretical Study of the Reaction of Carbonyl Oxide with Nitrogen Dioxide: CH ₂ OO + NO ₂ . <i>International Journal of Chemical Kinetics</i> , 2017, 49, 752-760.	1.0	25
8733	D2BIA–flexible, not (explicitly) arbitrary and reference/structurally invariant–a very effective and improved version of the D3BIA aromaticity index. <i>Journal of Molecular Modeling</i> , 2017, 23, 253.	0.8	3
8734	Elucidating Substrate Promiscuity within the FabI Enzyme Family. <i>ACS Chemical Biology</i> , 2017, 12, 2465-2473.	1.6	17

#	ARTICLE	IF	CITATIONS
8735	Time-Resolved Electron Paramagnetic Resonance and Theoretical Investigations of Metal-Free Room-Temperature Triplet Emitters. <i>Journal of the American Chemical Society</i> , 2017, 139, 12968-12975.	6.6	24
8736	Evaluation of photovoltaic properties and effective conjugated length of DTTD-based polymers as donor in BHJ solar cells; quantum chemical approach. <i>Polymer</i> , 2017, 126, 162-176.	1.8	19
8737	A low-cost approach to electronic excitation energies based on the driven similarity renormalization group. <i>Journal of Chemical Physics</i> , 2017, 147, 074107.	1.2	12
8738	Evaluating electronic structure methods for accurate calculation of ¹⁹ F chemical shifts in fluorinated amino acids. <i>Journal of Computational Chemistry</i> , 2017, 38, 2605-2617.	1.5	12
8739	Theoretical investigation of the structural, electronic, magnetic and spectral properties of CumXn (X) Tj ETQq0 0 0 igBT /Overlock 10 Tf	1.8	6
8740	Synthesis of Ferrocenyl-Based Unsymmetrical Azines via a Simple Reaction of Aldehydes with Ketone-Derived <i>N</i> -Tosyl Hydrazones and the Evaluation of the Extent of Conjugation in the Molecule. <i>Organometallics</i> , 2017, 36, 3215-3225.	1.1	9
8741	Spin-dependent charge recombination along para-phenylene molecular wires. <i>Journal of Chemical Physics</i> , 2017, 147, 064107.	1.2	13
8742	The Effect of Carboxamide/Sulfonamide Replacement in Arylpiperazinylalkyl Derivatives on Activity to Serotonin and Dopamine Receptors. <i>Archiv Der Pharmazie</i> , 2017, 350, 1700090.	2.1	5
8743	Practical Density Functionals beyond the Overdelocalizationâ€“Underbinding Zero-Sum Game. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4314-4318.	2.1	35
8744	A DFT Study on Palladium and Nickel-Catalyzed Regioselective and Stereoselective Hydrosilylation of 1,3-Disubstituted Allenes. <i>Organometallics</i> , 2017, 36, 3371-3381.	1.1	24
8745	Photoelectron spectroscopy of isolated luciferin and infraluciferin anions <i>in vacuo</i> : competing photodetachment, photofragmentation and internal conversion. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22711-22720.	1.3	14
8746	Triphenylamine-based fluorescent NLO phores with ICT characteristics: Solvatochromic and theoretical study. <i>Journal of Molecular Structure</i> , 2017, 1150, 493-506.	1.8	11
8747	Synthesis, DFT band structure calculations, optical and photoelectrical characterizations of the novel 5-hydroxy-4-methoxy-7-oxo-7H-furo[3,2-g]chromene-6-carbonitrile (HMOFCC). <i>Optical Materials</i> , 2017, 73, 290-305.	1.7	27
8748	The mechanism of excimer formation: an experimental and theoretical study on the pyrene dimer. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25002-25015.	1.3	119
8749	Fast construction of the exchange operator in an atom-centred basis with concentric atomic density fitting. <i>Molecular Physics</i> , 2017, 115, 2065-2076.	0.8	5
8750	New heterometallic pivalates with Fe III and Zn II ions: Synthesis, structures, magnetic, thermal properties. <i>Polyhedron</i> , 2017, 137, 165-175.	1.0	21
8751	Multireference Density Functional Theory with Generalized Auxiliary Systems for Ground and Excited States. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4479-4485.	2.1	21
8752	Star-Shaped Asymmetrically Substituted Blue Emitting Carbazoles: Synthesis, Photophysical, Electrochemical and Theoretical Investigations. <i>ChemistrySelect</i> , 2017, 2, 7514-7524.	0.7	11

#	ARTICLE	IF	CITATIONS
8753	A novel fluorescent sensor based on imidazole derivative for Fe ³⁺ ions. <i>Journal of Luminescence</i> , 2017, 192, 1096-1103.	1.5	27
8754	Why different ligands can control stereochemistry selectivity of Ni-catalyzed Suzuki-Miyaura cross-coupling of benzylic carbamates with arylboronic esters: a mechanistic study. <i>Dalton Transactions</i> , 2017, 46, 13010-13019.	1.6	14
8755	Theoretical study on structures and infrared spectroscopy of Cu ₂ (H ₂ O) _n (n = 1-4). <i>Russian Journal of Physical Chemistry A</i> , 2017, 91, 1752-1760.	0.1	0
8756	Dynamics of excited state proton transfer in nitro substituted 10-hydroxybenzo[h]quinolines. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26621-26629.	1.3	23
8757	Could the increased structural versatility imposed by non-halogen ligands bring something new for polynuclear superhalogens? A case study on binuclear [Mg ₂ L ₅] ⁺ (L = OH, OOH and OF) anions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26986-26995.	1.3	17
8758	Reactivity of Cyclic Silenolates Revisited. <i>Organometallics</i> , 2017, 36, 3765-3773.	1.1	8
8759	Dual Photochemical Reaction Pathway in Flavin-Based Photoreceptor LOV Domain: A Combined Quantum-Mechanics/Molecular-Mechanics Investigation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9583-9596.	1.2	14
8760	Bridge-driven aggregation control in dibenzofulvene-naphthalimide based donor-bridge-acceptor systems: enabling fluorescence enhancement, blue to red emission and solvatochromism. <i>Materials Chemistry Frontiers</i> , 2017, 1, 2590-2598.	3.2	19
8761	The Combination of Superhalogens and Brønsted Acids HX (X = F, Cl, Br): An Effective Strategy for Designing Strong Superacids. <i>Inorganic Chemistry</i> , 2017, 56, 11787-11797.	1.9	25
8762	Claisen rearrangements of benzyl vinyl ethers: theoretical investigation of mechanism, substituent effects, and regioselectivity. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 7887-7893.	1.5	7
8763	In Silico Test of Different Derivatives of Donor-Acceptor System To Realize Bipolar and Unipolar Spin Rectifier. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21695-21702.	1.5	4
8764	Molecular Engineering of Conjugated Polymers for Biocompatible Organic Nanoparticles with Highly Efficient Photoacoustic and Photothermal Performance in Cancer Theranostics. <i>ACS Nano</i> , 2017, 11, 10124-10134.	7.3	182
8765	Supramolecular complexes formed by dimethoxypillar[5]arenes and imidazolium salts: a joint experimental and computational investigation. <i>New Journal of Chemistry</i> , 2017, 41, 12490-12505.	1.4	4
8766	New Insights into the Catalytic Mechanism of Aldose Reductase: A QM/MM Study. <i>ACS Omega</i> , 2017, 2, 5737-5747.	1.6	8
8767	Extended screened exchange functional derived from transcorrelated density functional theory. <i>Journal of Chemical Physics</i> , 2017, 147, 104104.	1.2	3
8768	Comparative Study of Nonhybrid Density Functional Approximations for the Prediction of 3d Transition Metal Thermochemistry. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4907-4913.	2.3	30
8769	Projected Commutator DIIS Method for Accelerating Hybrid Functional Electronic Structure Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5458-5467.	2.3	21
8770	Self-Assembled Donor-Acceptor Chromophores: Evident Layer Effect on the First Hyperpolarizability and Two-Dimensional Charge Transfer Character. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21616-21626.	1.5	17

#	ARTICLE	IF	CITATIONS
8771	Ab Initio QM/MM Modeling of the Rate-Limiting Proton Transfer Step in the Deamination of Tryptamine by Aromatic Amine Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9785-9798.	1.2	16
8772	A study of size-dependent properties of MoS ₂ monolayer nanoflakes using density-functional theory. <i>Scientific Reports</i> , 2017, 7, 9775.	1.6	30
8773	Interplay between π -Bridges and Positions of Branched Alkyl Groups of Unsymmetrical D π -A π -A Squaraines in Dye-Sensitized Solar Cells: Mode of Dye Anchoring and the Charge Transfer Process at the TiO ₂ /Dye/Electrolyte Interface. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 32698-32712.	4.0	10
8774	Theoretical studies of spin state-specific [2+2] and [5+2] photocycloaddition reactions of <i>n</i> -pentenyl maleimide. <i>Journal of Computational Chemistry</i> , 2017, 38, 2388-2395.	1.5	2
8775	Real-time TD-DFT study on the dioxygen/superoxide radical charge transfer reaction. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 207-214.	1.1	5
8776	Assessment of Methodology and Chemical Group Dependences in the Calculation of the ρ -K _a for Several Chemical Groups. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4791-4803.	2.3	25
8777	Mechanistic investigation of the atmospheric reaction of NH ₂ with NO ₂ and study of the catalytic effects of water molecule on kinetic path. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750053.	1.8	2
8778	Winged-Cone Conformation in Hexa- <i>p</i> -tert-butylcalix[6]arene Driven by the Unusually Strong Guest Encapsulation. <i>ACS Omega</i> , 2017, 2, 5315-5323.	1.6	4
8779	A New Series of Highly Fluorescent Blue-Green Emitting, Imidazole-Based ICT-ESIPT Compounds: Detail Experimental and DFT Study of Structural and Donating Group Effects on Fluorescence Properties. <i>ChemistrySelect</i> , 2017, 2, 7691-7700.	0.7	19
8780	Protonation of Coordinated Dinitrogen Using Protons Generated from Molecular Hydrogen. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 4239-4245.	1.0	23
8781	Synergy of van der Waals and self-interaction corrections in transition metal monoxides. <i>Physical Review B</i> , 2017, 96, .	1.1	50
8782	Multinuclear σ -Staircase-Oligomers Based on the (Et ₂ C ₂ B ₄ H ₄)Fe(η^6 -C ₆ H ₆) Sandwich Unit: Quantitative Tailorable and Redox Switchable Nonlinear Optics. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16470-16480.	1.5	20
8783	Theoretical Investigation on Nickel-Catalyzed Hydrocarboxylation of Alkynes Employing Formic Acid. <i>Organometallics</i> , 2017, 36, 2818-2825.	1.1	24
8784	Temperature dependence of stable carbon kinetic isotope effect for the oxidation reaction of ethane by OH radicals: Experimental and theoretical studies. <i>Journal of Geophysical Research D: Atmospheres</i> , 2017, 122, 8310-8324.	1.2	2
8785	NMR spectroscopic conformational analysis of 4-methylene-cyclohexyl pivalate: The effect of sp ² hybridization. <i>Magnetic Resonance in Chemistry</i> , 2017, 55, 1073-1078.	1.1	0
8786	Pterocarpan and isoflavones from the root bark of <i>Millettia micans</i> and of <i>Millettia dura</i> . <i>Phytochemistry Letters</i> , 2017, 21, 216-220.	0.6	12
8787	Cycloaddition Reactions of Cobalt-Complexed Macrocyclic Alkynes: The Transannular Pauson-Khand Reaction. <i>Journal of Organic Chemistry</i> , 2017, 82, 7732-7744.	1.7	13
8788	Experimental and theoretical investigations of the gas adsorption sites in rht-metal-organic frameworks. <i>CrystEngComm</i> , 2017, 19, 4646-4665.	1.3	20

#	ARTICLE	IF	CITATIONS
8789	Effects of the substituents of pyrazole/thiazine ligands on the magnetic properties of chloro-bridged Cu(μ_2) complexes. <i>New Journal of Chemistry</i> , 2017, 41, 8818-8827.	1.4	8
8790	Excited state absorption spectra of dissolved and aggregated distyrylbenzene: A TD-DFT state and vibronic analysis. <i>Journal of Chemical Physics</i> , 2017, 147, 034903.	1.2	17
8791	<i>Ab initio</i> study of the lattice thermal conductivity of Cu_2O using the generalized gradient approximation and hybrid density functional methods. <i>Physical Review B</i> , 2017, 96, .	1.1	46
8792	A Complementary XRD and Theoretical Study of Water Induced Solid State Ionic Separation of Br^+ and Pyrazolium: A Case for Paradoxical Cation-Water Cluster. <i>ChemistrySelect</i> , 2017, 2, 5288-5291.	0.7	0
8793	Pericyclic or Pseudopericyclic? The Case of an Allylic Transposition in the Synthesis of a Saccharin Derivative. <i>Journal of Chemical Education</i> , 2017, 94, 988-993.	1.1	7
8794	[5 + 1 + 2 + 1] vs [5 + 1 + 1 + 2] Rhodium-Catalyzed Cycloaddition Reactions of Vinylcyclopropanes with Terminal Alkynes and Carbon Monoxide: Density Functional Theory Investigations of Convergent Mechanistic Pathways and Reaction Regioselectivity. <i>Organometallics</i> , 2017, 36, 2832-2842.	1.1	12
8796	Forsterite Surfaces as Models of Interstellar Core Dust Grains: Computational Study of Carbon Monoxide Adsorption. <i>ACS Earth and Space Chemistry</i> , 2017, 1, 384-398.	1.2	21
8797	Evaluating the electronic structure of formal Ln ^{II} ions in Ln ^{II} (C ₅ H ₄ SiMe ₃) ₃ using XANES spectroscopy and DFT calculations. <i>Chemical Science</i> , 2017, 8, 6076-6091.	3.7	42
8798	Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4535-4552.	2.3	90
8799	Trifluoromethylation of a Well-Defined Square-Planar Aryl-Ni ^{II} Complex involving Ni ^{III} /CF ₃ ⁺ and Ni ^{IV} CF ₃ Intermediate Species. <i>Chemistry - A European Journal</i> , 2017, 23, 11662-11668.	1.7	23
8800	Synthesis and Photophysical and Anion-Sensing Properties of Triarylborane-Substituted Cross-Conjugated and Conjugated Thienothiophenes. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 4552-4561.	1.2	38
8801	Experimental and theoretical studies on photoluminescent Zn(II) host complex with an open book structure: Implication on potential bioactivity and comparison with its ligand and Zn(II), Pd(II) siblings. <i>Polyhedron</i> , 2017, 135, 278-295.	1.0	19
8802	Calculations of σ^* Transition Energies: Comparisons Between TD-DFT, ADC, CC, CASPT2, and BSE/GW Descriptions. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6122-6134.	1.1	21
8803	Experimental and theoretical investigations of the kinetics and mechanism of the Cl ⁺ -4-hydroxy-4-methyl-2-pentanone reaction. <i>Atmospheric Environment</i> , 2017, 166, 315-326.	1.9	12
8804	Kinetics and mechanism of the reaction of recombination of vinyl and hydroxyl radicals. <i>Chemical Physics Letters</i> , 2017, 685, 165-170.	1.2	4
8805	Density Functional Theory Assessment of the Environment Polarity Effect on Polyaniline's "Water Coupling. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6327-6335.	1.1	1
8806	Spectroscopic Properties and Conformational Analysis of Methyl Ester of Sinapic Acid in Various Environments. <i>Journal of Physical Chemistry B</i> , 2017, 121, 7299-7310.	1.2	5
8807	DFT studies on the mechanism of Ag ₂ CO ₃ -catalyzed hydroazidation of unactivated terminal alkynes with TMS-N ₃ : An insight into the silver(I) activation mode. <i>Journal of Computational Chemistry</i> , 2017, 38, 2289-2297.	1.5	8

#	ARTICLE	IF	CITATIONS
8808	Multiscale Molecular Dynamics Simulations of Polaritonic Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4324-4335.	2.3	123
8809	Thermal isomerization of azobenzenes: on the performance of Eyring transition state theory. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 314002.	0.7	19
8810	[Au(9- <i>methylcaffein-8-ylidene</i>) ₂] ⁺ /DNA Tel23 System: Solution, Computational, and Biological Studies. <i>Chemistry - A European Journal</i> , 2017, 23, 13784-13791.	1.7	7
8811	4- <i>Electron N</i> Monocycles: Stability and (Anti)aromaticity. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 5163-5169.	1.2	10
8812	Theoretical prediction of noble gas inserted halocarbenes: FNgCX (Ng = Kr, and Xe; X = F, Cl, Br, and I). <i>Chemical Physics</i> , 2017, 494, 20-30.	0.9	13
8813	Bismuth nitrate-promoted disproportionative condensation of indoles with cyclohexanone: a new-type azafulvenium reactivity of indole. <i>New Journal of Chemistry</i> , 2017, 41, 9674-9687.	1.4	7
8814	Ab initio molecular dynamics study of the interaction of plutonium with oxygen in the gas phase. <i>RSC Advances</i> , 2017, 7, 36038-36047.	1.7	2
8815	Quantitative conformational stability host-guest complex of Carvacrol and Thymol with β -cyclodextrin: a theoretical investigation. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2017, 89, 143-155.	0.9	10
8816	The structure and C C vibrational frequencies of the all- trans polyenes C ₂ nH ₂ n+2 (n = 15), C ₂ nH ₂ n (Me) ₂ (n = 13), and C ₂ nH ₂ n (tert-Butyl) ₂ (n = 5): Computational results. <i>Chemical Data Collections</i> , 2017, 11-12, 25-35.		
8817	Atom Tunneling in the Water Formation Reaction H ₂ + OH → H ₂ O + H on an Ice Surface. <i>ACS Earth and Space Chemistry</i> , 2017, 1, 399-410.	1.2	38
8818	Spectroscopy and DFT Calculations of a Flavo-diiron Enzyme Implicate New Diiron Site Structures. <i>Journal of the American Chemical Society</i> , 2017, 139, 12009-12019.	6.6	32
8819	Relation between molecular electronic structure and nuclear spin-induced circular dichroism. <i>Scientific Reports</i> , 2017, 7, 46617.	1.6	6
8820	Magnetic circular dichroism and density functional theory studies of electronic structure and bonding in cobalt(ii)-N-heterocyclic carbene complexes. <i>Dalton Transactions</i> , 2017, 46, 13290-13299.	1.6	18
8821	Reactivity of the parent amido complexes of iridium with olefins: C-NH ₂ bond formation versus C-H activation. <i>Dalton Transactions</i> , 2017, 46, 11459-11468.	1.6	3
8822	Beryllium-based fluorenes as efficient anion sponges. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23052-23059.	1.3	10
8823	Fourth-order series expansion of the exchange hole. <i>Physical Review A</i> , 2017, 96, .	1.0	4
8824	Estimation of hydrophilicity of coals by using the quantum chemistry calculation. <i>International Journal of Mineral Processing</i> , 2017, 167, 9-15.	2.6	19
8825	Quantifying the Performances of DFT for Predicting Vibrationally Resolved Optical Spectra: Asymmetric Fluoroborate Dyes as Working Examples. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4347-4356.	2.3	18

#	ARTICLE	IF	CITATIONS
8826	Cyclopropyl Group: An Excited-State Aromaticity Indicator?. <i>Chemistry - A European Journal</i> , 2017, 23, 13684-13695.	1.7	10
8827	Investigating Intracellular Localisation and Cytotoxicity Trends for Neutral and Cationic Iridium Tetrazolato Complexes in Live Cells. <i>Chemistry - A European Journal</i> , 2017, 23, 15666-15679.	1.7	53
8828	Intramolecular interactions in sterically crowded hydrocarbon molecules. <i>Journal of Computational Chemistry</i> , 2017, 38, 2500-2508.	1.5	17
8829	Self-interaction effects on charge-transfer collisions. <i>Physical Review A</i> , 2017, 95, .	1.0	20
8830	Assessing accuracy of exchange-correlation functionals for electron affinities. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750052.	1.8	1
8831	Effect of Structure and Disorder on the Charge Transport in Defined Self-Assembled Monolayers of Organic Semiconductors. <i>ACS Nano</i> , 2017, 11, 8747-8757.	7.3	23
8832	Coordination and Thermodynamics of Trivalent Curium with Malonate at Increased Temperatures: A Spectroscopic and Quantum Chemical Study. <i>Inorganic Chemistry</i> , 2017, 56, 10172-10180.	1.9	9
8833	Magnetic-Field Density-Functional Theory (BDFT): Lessons from the Adiabatic Connection. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4089-4100.	2.3	32
8834	Protonation States of Homocitrate and Nearby Residues in Nitrogenase Studied by Computational Methods and Quantum Refinement. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8242-8262.	1.2	62
8835	Theoretical study of the substituent effect controlling the radiative and non-radiative decay processes of platinum(ii) complexes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23532-23540.	1.3	16
8836	Polycomplexes of the polycondensation products of boric acid and p-phenylenediamine. <i>Russian Journal of Physical Chemistry B</i> , 2017, 11, 499-503.	0.2	7
8837	On the structure of transition metals complexes with the new tridentate dye of thiazole series: Theoretical and experimental studies. <i>Journal of Molecular Structure</i> , 2017, 1149, 669-682.	1.8	33
8838	Description of ground and excited electronic states by ensemble density functional method with extended active space. <i>Journal of Chemical Physics</i> , 2017, 147, 064104.	1.2	27
8839	Efficient Phosphorescence from Naphthalenebenzimidazole-Coordinated Iridium(III) Chromophores. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 5238-5245.	1.0	14
8840	Comparison of classical reaction paths and tunneling paths studied with the semiclassical instanton theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23085-23094.	1.3	12
8841	Valence electronic structure of cobalt phthalocyanine from an optimally tuned range-separated hybrid functional. <i>Journal of Chemical Physics</i> , 2017, 147, 044301.	1.2	48
8842	Micro-solvation of tyrosine-kinase inhibitor AG1478 explored with fluorescence spectroscopy and computational chemistry. <i>RSC Advances</i> , 2017, 7, 31725-31735.	1.7	5
8843	Adsorption and coadsorption mechanisms of Cr(VI) and organic contaminants on H3PO4 treated biochar. <i>Chemosphere</i> , 2017, 186, 422-429.	4.2	133

#	ARTICLE	IF	CITATIONS
8844	Assessing Excited State Energy Gaps with Time-Dependent Density Functional Theory on Ru(II) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4123-4145.	2.3	39
8845	Unusual Role of Excited State Mixing in the Enhancement of Photoinduced Ligand Exchange in Ru(II) Complexes. <i>Journal of the American Chemical Society</i> , 2017, 139, 18295-18306.	6.6	23
8846	DFT/MRCI Hamiltonian for odd and even numbers of electrons. <i>Journal of Chemical Physics</i> , 2017, 147, 194104.	1.2	16
8847	Assessing the performance of self-consistent hybrid functional for band gap calculation in oxide semiconductors. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 454004.	0.7	33
8848	Theoretical study on the photophysical properties of boron-fused double helicenes. <i>RSC Advances</i> , 2017, 7, 56543-56549.	1.7	5
8849	Decomposition of Ionic Liquids at Lithium Interfaces. 1. <i>Ab Initio Molecular Dynamics Simulations</i> . <i>Journal of Physical Chemistry C</i> , 2017, 121, 28214-28234.	1.5	68
8850	Aromaticity-Driven Molecular Structural Variation and Electronic Configuration Alternation: An Example of Cyclic π Conjugation Involving a Mo σ -Mo π Bond. <i>Inorganic Chemistry</i> , 2017, 56, 14888-14899.	1.9	4
8851	Planar Octagonal Tetranuclear Cobaltacarborane Macrocycle [(μ - ⁵ -C ₅ Me ₅)Co(2,3-Et ₂ C ₂ B ₄ H ₃ -5-C σ)] ₂ for 2D Nonlinear Optics: Ultra-High-Response and Multistate Controlled Cubic NLO Switch. <i>Journal of Physical Chemistry C</i> , 2017, 121, 28462-28474.	1.5	19
8852	Understanding the interplay between the solvent and nuclear rearrangements in the negative solvatochromism of a push π -pull flexible quinolinium cation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32544-32555.	1.3	7
8853	Hybrid complex polymers of boron and imidazole hydroxide. <i>Russian Journal of Physical Chemistry B</i> , 2017, 11, 839-845.	0.2	8
8854	Tunneling Rate Constants for H ₂ CO+H on Amorphous Solid Water Surfaces. <i>Astrophysical Journal</i> , 2017, 850, 118.	1.6	26
8855	The Atmospheric Oxidation of HONO by OH, Cl, and ClO Radicals. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9698-9707.	1.1	15
8856	Spectral and quantum-mechanical characterizations of 7-amino-4-trifluoromethyl coumarin. <i>AIP Conference Proceedings</i> , 2017, .	0.3	1
8857	A note on the accuracy of KS-DFT densities. <i>Journal of Chemical Physics</i> , 2017, 147, 204103.	1.2	23
8858	Theoretical calculation pKa values of phthalhydrazide derivatives in its aqueous solutions. <i>Russian Journal of Physical Chemistry B</i> , 2017, 11, 722-728.	0.2	4
8859	Electronic Structure of Anilinopyridinate-Supported Ru ₂ ⁺⁵ Paddlewheel Compounds. <i>Inorganic Chemistry</i> , 2017, 56, 14662-14670.	1.9	13
8860	Seeking an accurate generalized-gradient approximation functional for high pressure molecular fluids. <i>Journal of Applied Physics</i> , 2017, 122, .	1.1	8
8861	Redox-dependent properties of DTF-encapped π -oligomers. <i>New Journal of Chemistry</i> , 2017, 41, 15251-15259.	1.4	3

#	ARTICLE	IF	CITATIONS
8862	Competitive/co-operative interactions in acid base sandwich: role of cation vs. substituents. <i>Journal of Molecular Modeling</i> , 2017, 23, 341.	0.8	1
8863	Does alkali cation binding to aromatic ring retard the fluxional haptotropic migration? Evidences from density functional study. <i>Journal of Chemical Sciences</i> , 2017, 129, 1843-1851.	0.7	0
8864	Circular cationic compounds B ₃ Rgn ⁺ of triangular ion B ₃ ⁺ trapping rare gases. <i>Chemical Research in Chinese Universities</i> , 2017, 33, 958-964.	1.3	1
8865	Localized Intrinsic Valence Virtual Orbitals as a Tool for the Automatic Classification of Core Excited States. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5984-5999.	2.3	9
8866	A computational investigation of the solvent-dependent enantioselective intramolecular Morita-Baylis-Hillman reaction of enones. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 10212-10220.	1.5	9
8868	A Zn(II)-Containing Coordination Polymer: Synthesis, Crystal Structure and pH Fluorescent Sensing. <i>Crystal Research and Technology</i> , 2017, 52, 1700105.	0.6	8
8869	Lighting up long-range charge-transfer states by a localized plasmonic field. <i>Nanoscale</i> , 2017, 9, 18189-18193.	2.8	14
8870	Computational Plasmonics: Numerical Techniques. <i>Springer Series in Optical Sciences</i> , 2017, , 341-368.	0.5	3
8871	How Well Can the M06 Suite of Functionals Describe the Electron Densities of Ne, Ne ⁶⁺ , and Ne ⁸⁺ ?. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6068-6077.	2.3	25
8872	QM/MM Study of the Conversion of Oxophlorin into Verdoheme by Heme Oxygenase. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11427-11436.	1.2	9
8873	Two-dimensional van der Waals heterojunctions for functional materials and devices. <i>Journal of Materials Chemistry C</i> , 2017, 5, 12289-12297.	2.7	151
8874	Determination of trace metal concentration in compost, DAP, and TSP fertilizers by neutron activation analysis (NAA) and insights from density functional theory calculations. <i>Environmental Monitoring and Assessment</i> , 2017, 189, 618.	1.3	10
8875	Experimental-Computational Synergy for Selective Pd(II)-Catalyzed C-H Activation of Aryl and Alkyl Groups. <i>Accounts of Chemical Research</i> , 2017, 50, 2853-2860.	7.6	189
8876	(Oligo-)Thiophene Functionalized Tetraazaperopyrenes: Donor-Acceptor Dyes and Ambipolar Organic Semiconductors. <i>Journal of Organic Chemistry</i> , 2017, 82, 12492-12502.	1.7	19
8877	The Hydrogen Abstraction Reaction H ₂ S + OH → H ₂ O + SH: Convergent Quantum Mechanical Predictions. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9136-9145.	1.1	11
8878	Mechanistic Studies of Redox-Switchable Copolymerization of Lactide and Cyclohexene Oxide by a Zirconium Complex. <i>Organometallics</i> , 2017, 36, 4451-4457.	1.1	36
8879	Floppy molecules as candidates for achieving optoelectronic molecular devices without skeletal rearrangement or bond breaking. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30842-30851.	1.3	13
8880	Ultrafast 25-fs relaxation in highly excited states of methyl azide mediated by strong nonadiabatic coupling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E11072-E11081.	3.3	13

#	ARTICLE	IF	CITATIONS
8881	A study of accurate exchange-correlation functionals through adiabatic connection. <i>Journal of Chemical Physics</i> , 2017, 147, 144105.	1.2	9
8882	Symmetry breaking in occupation number based slave-particle methods. <i>Physical Review B</i> , 2017, 96, .	1.1	8
8883	Methane Adsorption in Zr-Based MOFs: Comparison and Critical Evaluation of Force Fields. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25309-25322.	1.5	34
8884	Justifying quasiparticle self-consistent schemes via gradient optimization in Baym's Kadanoff theory. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 385501.	0.7	15
8885	Triphenylamine-Based Bis- and Tris-ESIPT Compounds and Their Boron Complexes: Synthesis, Photophysical Properties and DFT Study of ICT and ESIPT Emissions. <i>ChemistrySelect</i> , 2017, 2, 5013-5024.	0.7	10
8886	Solvatochromic benzo[h] coumarins: Synthesis, solvatochromism, NLO and DFT study. <i>Optical Materials</i> , 2017, 72, 346-358.	1.7	20
8887	A quantum-mechanical model of dilatation dipoles in topochemical synthesis of silicon carbide from silicon. <i>Physics of the Solid State</i> , 2017, 59, 1238-1241.	0.2	3
8888	Diastereoselective Self-Assembly of a Neutral Dinuclear Double-Stranded Zinc(II) Helicate via Narcissistic Self-Sorting. <i>Chemistry - A European Journal</i> , 2017, 23, 12380-12386.	1.7	18
8889	TD-DFT calculations, NBO analysis and electronic absorption spectra of some thiazolo[3,2-a]pyridine derivatives. <i>Journal of Molecular Structure</i> , 2017, 1147, 651-667.	1.8	31
8890	Experimental Determination of the Molar Absorption Coefficient of <i>n</i> -Hexane Adsorbed on High-Silica Zeolites. <i>ChemPhysChem</i> , 2017, 18, 2374-2380.	1.0	6
8891	A Two-Coordinate Neutral Germylene Supported by a λ^2 -Diketiminato Ligand in the Radical State. <i>Organometallics</i> , 2017, 36, 2706-2709.	1.1	27
8892	Ionization energies and electron affinities from a random-phase-approximation many-body Green's-function method including exchange interactions. <i>Physical Review A</i> , 2017, 95, .	1.0	8
8893	4,4'-Di-tert-butyl-6-(1H-tetrazol-5-yl)-2,2'-bipyridine: modification of a highly selective N-donor ligand for the separation of trivalent actinides from lanthanides. <i>Dalton Transactions</i> , 2017, 46, 9981-9994.	1.6	15
8894	The effect of $[D_{e/n}]^{\text{A}}_{n/n}$ ($n = 1, 2, 3$) type dyes on the overall performance of DSSCs: a theoretical investigation. <i>Journal of Materials Chemistry C</i> , 2017, 5, 7510-7520.	2.7	22
8895	Systematic Functional Analysis of Active-Site Residues in <i>Thermoplasma volcanium</i> -Threonine Dehydrogenase from <i>Thermoplasma volcanium</i> . <i>ACS Omega</i> , 2017, 2, 3308-3314.	1.6	3
8896	Effect of Rigid Bridge-Protection Units, Quadrupolar Interactions, and Blending in Organic Electro-Optic Chromophores. <i>Chemistry of Materials</i> , 2017, 29, 6457-6471.	3.2	76
8897	Hydroxyl radical-mediated degradation of diclofenac revisited: a computational approach to assessment of reaction mechanisms and by-products. <i>Environmental Science and Pollution Research</i> , 2017, 24, 18458-18469.	2.7	25
8898	Azafluorene Ornamented Thiazine Based Novel Fused Heterocyclic Organic Dyes for Competent Molecular Photovoltaics. <i>Electrochimica Acta</i> , 2017, 246, 1052-1064.	2.6	15

#	ARTICLE	IF	CITATIONS
8899	What Is the Optoelectronic Effect of the Capsule on the Guest Molecule in Aqueous Host/Guest Complexes? A Combined Computational and Spectroscopic Perspective. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15481-15488.	1.5	17
8900	Solvatochromic and Quantum-Mechanical Characterization of Methyl Red. <i>Analytical Letters</i> , 2017, 50, 2711-2724.	1.0	3
8901	Full-valence density matrix renormalisation group calculations on meta-benzyne based on unrestricted natural orbitals. Revisit of seamless continuation from broken-symmetry to symmetry-adapted models for diradicals. <i>Molecular Physics</i> , 2017, 115, 2267-2284.	0.8	14
8902	The application of TD-DFT to excited states of a family of TPD molecules interesting for optoelectronic use. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	2
8903	Time-evolution study of photoinduced charge-transfer in tertiary amine-fluorophore systems. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 197-207.	1.1	5
8904	Weakening of Si Si bonding in exohydrogenated Si ₆₀ nanoclusters. <i>Chemical Physics Letters</i> , 2017, 684, 60-66.	1.2	1
8905	Biophysical studies on the interaction of a novel oxime based palladium(II) complex with DNA and RNA. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2017, 173, 560-570.	1.7	22
8906	NLOphoric donor-rigidified ESIPT dyes – Synthesis, pH study, solvatochromism and DFT insights. <i>Journal of Luminescence</i> , 2017, 192, 343-358.	1.5	9
8907	Generation and Characterization of Gas-Phase Doubly Charged Biradical Peptide Ions (M ²⁺). <i>Analytical Chemistry</i> , 2017, 89, 7773-7780.	3.2	2
8908	Isoflavones and Rotenoids from the Leaves of <i>Millettia oblata</i> ssp. <i>teitensis</i> . <i>Journal of Natural Products</i> , 2017, 80, 2060-2066.	1.5	28
8909	Quantum Chemical Investigation on Photochemical Reactions of Nonanoic Acids at Air–Water Interface. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4253-4262.	1.1	9
8910	Comparison of DFT functionals for prediction of band gap of conjugated polymers and effect of HF exchange term percentage and basis set on the performance. <i>Computational Materials Science</i> , 2017, 138, 70-76.	1.4	48
8911	A theoretical study of the low-lying excited states and the photophysics of dimethoxy curcumin in cyclohexane and acetonitrile. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	0
8912	Computational Studies of Substituted Phenylboronic Acids in Common Electrolyte Solvents. <i>Arabian Journal for Science and Engineering</i> , 2017, 42, 4227-4238.	1.7	2
8913	Electronic structure of $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{Pr} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle 1 \langle \text{mml:mi} \rangle$. <i>Physical Review B</i> , 2017, 95, .	1.1	1
8914	Acetylcholinesterase inhibitory assessment of isolated constituents from <i>Salsola grandis</i> Freitag, Vural & Adigüzel and molecular modeling studies on N-acetyltryptophan. <i>Phytochemistry Letters</i> , 2017, 20, 373-378.	0.6	23
8915	Polydopamine and eumelanin molecular structures investigated with ab initio calculations. <i>Chemical Science</i> , 2017, 8, 1631-1641.	3.7	162
8916	The mechanistic and kinetic investigation on the atmospheric reaction of atomic O(3P) with crotonitrile. <i>Computational and Theoretical Chemistry</i> , 2017, 1099, 140-151.	1.1	1

#	ARTICLE	IF	CITATIONS
8917	DFT study of nitrogen monoxide adsorption and dissociation on Rh Cu nano clusters. Journal of Alloys and Compounds, 2017, 695, 1924-1929.	2.8	7
8918	Inactivation of urease by catechol: Kinetics and structure. Journal of Inorganic Biochemistry, 2017, 166, 182-189.	1.5	57
8919	Charge-transfer contributions to the excitonic coupling matrix element in BODIPY-based energy transfer cassettes. Chemical Physics, 2017, 482, 265-276.	0.9	16
8920	Experimental and theoretical studies on electropolymerization of polar amino acids on platinum electrode. Materials Chemistry and Physics, 2017, 185, 183-194.	2.0	16
8921	Putative biosynthetic cycloadditions en route to the diterpenoid (+)-chatancin. Tetrahedron, 2017, 73, 4227-4232.	1.0	6
8922	How reliable is DFT in predicting relative energies of polycyclic aromatic hydrocarbon isomers? comparison of functionals from different rungs of Jacob's ladder. Journal of Computational Chemistry, 2017, 38, 370-382.	1.5	43
8923	Stability of the chlorinated derivatives of the DNA/RNA nucleobases, purine and pyrimidine toward radical formation via homolytic C-Cl bond dissociation. International Journal of Quantum Chemistry, 2017, 117, e25319.	1.0	8
8924	A DFT study of the interaction between large PAHs and atomic chlorine or hydrogen chloride molecule: Toward a modelling of the influence of chlorinated species on the trapping of water by soot. Chemical Physics, 2017, 483-484, 46-55.	0.9	3
8925	Nucleophilic aromatic substitution in chlorinated aromatic systems with a glutathione thiolate model. Journal of Physical Organic Chemistry, 2017, 30, e3640.	0.9	2
8926	Novel Thiazole Based Styryl Dyes with Benzimidazole Unit - Synthesis, Photophysical and TD-DFT Studies. Journal of Fluorescence, 2017, 27, 167-180.	1.3	8
8927	A computational investigation on the influence of different spacer groups in the bithiazole-based organic dye sensitizers on the short-circuit photocurrent densities of dye-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 333, 70-78.	2.0	23
8928	Synthesis, DFT calculations, electronic structure, electronic absorption spectra, natural bond orbital (NBO) and nonlinear optical (NLO) analysis of the novel 5-methyl-8H-benzo[h]chromeno[2,3-b][1,6] naphthyridine-6(5H),8-dione (MBCND). Journal of Molecular Structure, 2017, 1130, 543-558.	1.8	44
8929	The influence of structural factors on the composition, spectral-luminescent properties and thermal stability of zinc(II) bis(dipyrromethene)s crystal solvates with amines. Journal of Molecular Structure, 2017, 1130, 385-394.	1.8	8
8930	Theoretical study of zinc porphyrin-based dyes for dye-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 333, 200-207.	2.0	12
8931	Photochemical and DFT studies on DNA-binding ability and antibacterial activity of lanthanum(III)-phenanthroline complex. Journal of Molecular Structure, 2017, 1130, 940-950.	1.8	32
8932	³¹ P-Solid-State NMR Characterization and Catalytic Hydrogenation Tests of Novel heterogenized Iridium-Catalysts. Zeitschrift Fur Physikalische Chemie, 2017, 231, 653-669.	1.4	9
8933	Cryptic post-transition state bifurcations that reduce the efficiency of lactone-forming Rh-carbenoid C-H insertions. Chemical Science, 2017, 8, 1442-1449.	3.7	69
8934	Solvent effect on the tautomers' stabilities of protonated N,N-dimethylnitrosamine: The role of hydrogen bonds network. International Journal of Quantum Chemistry, 2017, 117, e25311.	1.0	1

#	ARTICLE	IF	CITATIONS
8935	Reactivity, vibrational spectroscopy, internal rotation and thermochemical aspects of methylarsine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 171, 383-394.	2.0	9
8936	Insight into opto-electronic property by modifying optical layers with multi-polar and multi-branched structures. <i>Journal of Materials Science: Materials in Electronics</i> , 2017, 28, 1489-1500.	1.1	4
8937	The adsorption and dissociation of water molecule on goethite (010) surface: A DFT approach. <i>Applied Surface Science</i> , 2017, 392, 760-767.	3.1	30
8938	Donor- and acceptor-functionalized dibenzo[a,e]pentalenes: modulation of the electronic band gap. <i>Organic Chemistry Frontiers</i> , 2017, 4, 658-663.	2.3	39
8939	A systematic study of phenoxazine-based organic sensitizers for solar cells. <i>Dyes and Pigments</i> , 2017, 137, 12-23.	2.0	61
8940	The Magnetic Transition of Tcn ($n\hat{A}=1, 2$) Induced by the Reaction with Cl and BO ₂ . <i>Journal of Cluster Science</i> , 2017, 28, 905-915.	1.7	0
8941	A computational study of ion speciation in mixtures of protic ionic liquids with various molecular solvents: Insight into the solvent polarity and anion basicity. <i>International Journal of Quantum Chemistry</i> , 2017, 117, 170-179.	1.0	4
8942	Effect of the species and number of heteroatom on the interaction energy and charge transfer between crown ether and alkali metal ions. <i>Structural Chemistry</i> , 2017, 28, 749-756.	1.0	3
8943	Pyrrole-thiazole based push-pull chromophores: An experimental and theoretical approach to structural, spectroscopic and NLO properties of the novel styryl dyes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 333, 1-17.	2.0	34
8944	Hydrogen-adduction to open-shell graphene fragments: spectroscopy, thermochemistry and astrochemistry. <i>Chemical Science</i> , 2017, 8, 1186-1194.	3.7	6
8945	Copper(I)-catalyzed reaction of unsymmetrical alkyne with HB($\langle\text{sc}\rangle\text{pin}\langle/\text{sc}\rangle$): a density functional theory study. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3630.	0.9	3
8946	Synthesis, characterization, density functional study and antimicrobial evaluation of a series of bischelated complexes with a dithiocarbamate Schiff base ligand. <i>Arabian Journal of Chemistry</i> , 2017, 10, 172-184.	2.3	27
8947	Are there reliable DFT approaches for ^{13}C NMR chemical shift predictions of fullerene C ₆₀ derivatives?. <i>International Journal of Quantum Chemistry</i> , 2017, 117, 7-14.	1.0	11
8948	A combined spectroscopic and TDDFT study of natural dyes extracted from fruit peels of <i>Citrus reticulata</i> and <i>Musa acuminata</i> for dye-sensitized solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 171, 112-125.	2.0	39
8949	Viability of dodecahedrane-forming radical polycyclizations. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 1976-1979.	1.5	4
8950	The removal of Basic Blue 41 textile dye from aqueous solution by adsorption onto natural zeolitic tuff: Kinetics and thermodynamics. <i>Chemical Engineering Research and Design</i> , 2017, 105, 274-287.	2.7	93
8951	Molecular modeling guided isotope separation of gadolinium with strong cation exchange resin using displacement chromatography. <i>Separation Science and Technology</i> , 2017, 52, 2300-2307.	1.3	7
8952	Carbon Nanotubes Covalently Attached to Functionalized Surfaces Directly through the Carbon Cage. <i>Langmuir</i> , 2017, 33, 1121-1131.	1.6	11

#	ARTICLE	IF	CITATIONS
8953	A Thiosemicarbazoneâ€“Nickel(II) Complex as Efficient Electrocatalyst for Hydrogen Evolution. <i>ChemCatChem</i> , 2017, 9, 2262-2268.	1.8	57
8954	Potentiality of Density-Functional Theory in Analyzing the Devices Containing Graphene-Crystalline Solid Interfaces: A Review. <i>IEEE Transactions on Electron Devices</i> , 2017, 64, 4738-4745.	1.6	8
8955	Synthesis, characterization and photophysical properties of ferrocenyl and mixed sandwich cobaltocenyl ester linked <i>meso</i> -triaryl corrole dyads. <i>Journal of Porphyrins and Phthalocyanines</i> , 2017, 21, 646-657.	0.4	2
8956	The DNA-binding behavior and DFT calculation of ruthenium(II) complexes [Ru(phen)2L](ClO4)2 (L = Tj ETQq1 1 0,784314 rgBT /Ove	0.8	0
8957	A pH-induced conformational switch in a tyrosine kinase inhibitor identified by electronic spectroscopy and quantum chemical calculations. <i>Scientific Reports</i> , 2017, 7, 16271.	1.6	3
8958	When combined X-ray and polarized neutron diffraction data challenge high-level calculations: spin-resolved electron density of an organic radical. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 544-549.	0.5	13
8959	Spectroscopic detection of halogen bonding resolves dye regeneration in the dye-sensitized solar cell. <i>Nature Communications</i> , 2017, 8, 1761.	5.8	35
8960	Novel type ketone-substituted metallophthalocyanines: synthesis, spectral, structural, computational and anticancer studies. <i>RSC Advances</i> , 2017, 7, 56296-56305.	1.7	27
8961	rPM6 Parameters for Manganese and Application to Transition State Search for Oxidation Reactions of Cyclohexene by Manganese(IV)-Oxo Species. <i>Chemistry Letters</i> , 2017, 46, 1567-1569.	0.7	3
8962	Molecular engineering of functionalized crown ether resins for the isotopic enrichment of gadolinium: from computer to column chromatography. <i>Molecular Systems Design and Engineering</i> , 2017, 2, 640-652.	1.7	9
8963	Hexagonal boron cluster as an anode material for divalent-ion (Ca ²⁺) storage: A theoretical study. , 2017, , .		0
8964	Tetranuclear Ni(<i>ii</i>) and Co(<i>ii</i>) Schiff-base complexes with an M ₄ O ₆ defective dicubane-like core: zero-field SMM behavior in the cobalt analogue. <i>New Journal of Chemistry</i> , 2017, 41, 11258-11267.	1.4	34
8965	Thermal Stability of Heptaprismane C ₁₄ H ₁₄ . <i>Journal of Physics: Conference Series</i> , 2017, 938, 012070.	0.3	0
8966	Biological activities of triazine derivatives. Combining DFT and QSAR results. <i>Arabian Journal of Chemistry</i> , 2017, 10, S946-S955.	2.3	28
8967	Exploring the Interactions of Atomic Oxygen on Silver Clusters with Hydrogen. <i>Chinese Journal of Chemical Physics</i> , 2017, 30, 685-690.	0.6	2
8968	Theoretical investigation of the Structure Activity Relationships (SARs) of a series of five isomeric $\hat{1}$, $\hat{2}$, $\hat{3}$, $\hat{4}$, $\hat{5}$ ruthenium complexes RuCl ₂ L ₂ with azopyridine ligands [L= azpy, tazpy, 4mazpy, 5mazpy]. <i>International Journal of Engineering Research and Applications</i> , 2017, 07, 58-70.	0.1	1
8969	Exploration of the Structural, Electronic and Tunable Magnetic Properties of Cu ₄ M (M = Sc-Ni) Clusters. <i>Materials</i> , 2017, 10, 946.	1.3	5
8970	Nonempirical Simulations of Inhomogeneous Broadening of Electronic Transitions in Solution: Predicting Band Shapes in One- and Two-Photon Absorption Spectra of Chalcones. <i>Molecules</i> , 2017, 22, 1643.	1.7	15

#	ARTICLE	IF	CITATIONS
8971	Asymmetric bioreduction of α^2 -ketoesters derivatives by <i>Kluyveromyces marxianus</i> : influence of molecular structure on the conversion and enantiomeric excess. <i>Anais Da Academia Brasileira De Ciencias</i> , 2017, 89, 1403-1415.	0.3	9
8972	Level of Theory and Solvent Effects on DASA Absorption Properties Prediction: Comparing TD-DFT, CASPT2 and NEVPT2. <i>Materials</i> , 2017, 10, 1025.	1.3	22
8973	First-Principles View on Photoelectrochemistry: Water-Splitting as Case Study. <i>Inorganics</i> , 2017, 5, 37.	1.2	22
8974	The Silacyclobutene Ring: An Indicator of Triplet State Baird-Aromaticity. <i>Inorganics</i> , 2017, 5, 91.	1.2	5
8975	Excited-State Dynamics of the Thiopurine Prodrug 6-Thioguanine: Can N9-Glycosylation Affect Its Phototoxic Activity?. <i>Molecules</i> , 2017, 22, 379.	1.7	43
8976	Intramolecular Hydrogen Bonding and Conformational Preferences of Arzanolâ€”An Antioxidant Acylphloroglucinol. <i>Molecules</i> , 2017, 22, 1294.	1.7	23
8977	A Theoretical Study of the N to O Linkage Photoisomerization Efficiency in a Series of Ruthenium Mononitrosyl Complexes. <i>Molecules</i> , 2017, 22, 1667.	1.7	8
8978	ORGANIC NITROGEN CONVERSION DURING THE THERMAL DECOMPOSITION OF HUADIAN OIL SHALE OF CHINA. <i>Oil Shale</i> , 2017, 34, 97.	0.5	5
8979	First Principle Modelling of Materials and Processes in Dye-Sensitized Photoanodes for Solar Energy and Solar Fuels. <i>Computation</i> , 2017, 5, 5.	1.0	15
8980	New Abietane and Kaurane Type Diterpenoids from the Stems of <i>Tripterygium regelii</i> . <i>International Journal of Molecular Sciences</i> , 2017, 18, 147.	1.8	13
8981	DFT-based Theoretical Simulations for Photocatalytic Applications Using TiO ₂ . , 0, , .		3
8982	Torsional Potential Energy Surfaces of Dinitrobenzene Isomers. <i>Advances in Condensed Matter Physics</i> , 2017, 2017, 1-7.	0.4	1
8983	Importance of the Inter-Electrode Distance for the Electrochemical Synthesis of Magnetite Nanoparticles: Synthesis, Characterization, Computational Modelling, and Cytotoxicity. <i>E-Journal of Surface Science and Nanotechnology</i> , 2017, 15, 31-39.	0.1	27
8984	Technologically Relevant Applications. , 2017, , 335-386.		0
8985	Prediction of Fundamental Properties of Semiconductors and Materials Exploration Using First-Principles Calculations. <i>Materia Japan</i> , 2017, 56, 554-559.	0.1	0
8986	Infrared Investigations of the Neutral-Ionic Phase Transition in TTF-CA and Its Dynamics. <i>Crystals</i> , 2017, 7, 17.	1.0	15
8987	Wavefunction Theory Approaches to Noncovalent Interactions. , 2017, , 137-168.		4
8988	Electronic Structures, and Optical and Magnetic Properties of Quadruple-Decker Phthalocyanines. <i>Magnetochemistry</i> , 2017, 3, 21.	1.0	2

#	ARTICLE	IF	CITATIONS
8989	The Exchange-Hole Dipole Moment Dispersion Model. , 2017, , 169-194.		37
8990	Asymmetric synthesis, molecular modeling and biological evaluation of 5-methyl-3-aryloxazolidine-2,4-dione enantiomers as monoamine oxidase (MAO) inhibitors. <i>Bioorganic Chemistry</i> , 2018, 77, 608-618.	2.0	14
8991	Structural and spectrophotometric characterization of 2-[4-(dimethylamino)styryl]-1-ethylquinolinium iodide as a reagent for sequential injection determination of tungsten. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 196, 398-405.	2.0	19
8992	Copper Nanoparticles in Polyvinyl Alcohol–Acrylic Acid Matrix: An Efficient Heterogeneous Catalyst for the Regioselective Synthesis of 1,4-Disubstituted 1,2,3-Triazoles via Click Reaction. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2018, 28, 1457-1467.	1.9	18
8994	Toward Accurate Conformational Energies of Smaller Peptides and Medium-Sized Macrocycles: MPCONF196 Benchmark Energy Data Set. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1254-1266.	2.3	69
8995	Optimization of long range potential interaction parameters in ion mobility spectrometry. <i>Journal of Chemical Physics</i> , 2018, 148, 074102.	1.2	33
8996	ONIOM and FMO–EDA study of metabotropic glutamate receptor 1: Quantum insights into the allosteric binding site. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25617.	1.0	6
8997	S-doped mesoporous graphene microspheres: A high performance reservoir material for Li S batteries. <i>Electrochimica Acta</i> , 2018, 269, 83-92.	2.6	46
8998	Exploration of Uncharted ³ PES Territory for [Ru(bpy) ₃] ²⁺ : A New ³ MC Minimum Prone to Ligand Loss Photochemistry. <i>Inorganic Chemistry</i> , 2018, 57, 3192-3196.	1.9	30
8999	Examining the Ways To Bend and Break Reaction Pathways Using Mechanochemistry. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6996-7004.	1.5	20
9000	Phosphole–Thiophene Hybrid: A Dual Role of Dithieno[3,4- <i>b</i> :3′,4′- <i>d</i>]phosphole as Electron Acceptor and Electron Donor. <i>Journal of Organic Chemistry</i> , 2018, 83, 3397-3402.	1.7	12
9001	Post-B3LYP Functionals Do Not Improve the Description of Magnetic Coupling in Cu(II) Dinuclear Complexes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3423-3432.	1.1	12
9002	Assessment of Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) in Radiation Chemistry: Ionized Water Dimer. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3227-3237.	1.1	24
9003	Predicting Productive Binding Modes for Substrates and Carbocation Intermediates in Terpene Synthases—Bornyl Diphosphate Synthase As a Representative Case. <i>ACS Catalysis</i> , 2018, 8, 3322-3330.	5.5	34
9004	Electronic structure and luminescence properties of unique complexes: cyclometalated iridium(III) chelated by <i>o</i> -carboranyl-pyridine ligands. <i>New Journal of Chemistry</i> , 2018, 42, 5955-5966.	1.4	5
9005	The pH-dependent activation mechanism of Ser102 in Escherichia coli alkaline phosphatase: a theoretical study. <i>Journal of Biological Inorganic Chemistry</i> , 2018, 23, 277-284.	1.1	9
9006	Mechanistic insights into asymmetric reductive coupling of isoquinolines by a chiral diboron with DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 97-104.	0.8	13
9007	Prediction of ¹⁹ F NMR Chemical Shifts for Fluorinated Aromatic Compounds. <i>Journal of Organic Chemistry</i> , 2018, 83, 3220-3225.	1.7	31

#	ARTICLE	IF	CITATIONS
9008	Structure-efficiency relationship of newly synthesized 4-substituted donor-acceptor coumarins for dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2018, 42, 5267-5275.	1.4	40
9009	Theoretical insight into the substituent effects on the antioxidant properties of 8-hydroxyquinoline derivatives in gas phase and in polar solvents. <i>Canadian Journal of Chemistry</i> , 2018, 96, 453-458.	0.6	3
9010	Experimental and computational study on the electrochemistry of meso-tetrasubstituted porphyrins: Effects of resonance and inductive substituents. <i>Journal of Electroanalytical Chemistry</i> , 2018, 815, 40-46.	1.9	3
9011	Structural and spectroscopic characterization, reactivity study and charge transfer analysis of the newly synthesized 2-(6-hydroxy-1-benzofuran-3-yl) acetic acid. <i>Journal of Molecular Structure</i> , 2018, 1162, 81-95.	1.8	11
9012	Synthesis, Characterization, and Reactivity of a <i>High-Spin</i> Iron(II) Hydrido Complex Supported by a PNP Pincer Ligand and Its Application as a Homogenous Catalyst for the Hydrogenation of Alkenes. <i>Inorganic Chemistry</i> , 2018, 57, 3183-3191.	1.9	35
9013	Unimolecular Fragmentation of Deprotonated Diproline [Pro ₂ -H] ⁺ Studied by Chemical Dynamics Simulations and IRMPD Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2612-2625.	1.1	18
9014	Time-dependent broken-symmetry density functional theory simulation of the optical response of entangled paramagnetic defects: Color centers in lithium fluoride. <i>Physical Review B</i> , 2018, 97, .	1.1	3
9015	DFT study of the infrared and Raman spectra of photochromic Fulgide;		

#	ARTICLE	IF	CITATIONS
9026	Electronic structure of phosphorene nanoflakes. A theoretical insight. Computational and Theoretical Chemistry, 2018, 1130, 33-45.	1.1	4
9027	A highly selective fluorescent probe for cyanide ion and its detection mechanism from theoretical calculations. Talanta, 2018, 185, 1-6.	2.9	28
9028	Third-Order Nonlinear Optical Properties of Endohedral Fullerene (H ₂) ₂ @C ₇₀ and (H ₂ O) ₂ @C ₇₀ Accompanied by the Prospective of Novel (HF) ₂ @C ₇₀ . Journal of Physical Chemistry C, 2018, 122, 6835-6845.	1.5	24
9029	Acid-Free Conversion of Cellulose to 5-(Hydroxymethyl)furfural Catalyzed by Hot Seawater. Industrial & Engineering Chemistry Research, 2018, 57, 3545-3553.	1.8	61
9030	Large Negative Differential Resistance and Rectification from a Donor-“f”-Acceptor Molecule in the Presence of Dissimilar Electrodes. Chemistry - A European Journal, 2018, 24, 5876-5882.	1.7	4
9031	Functionalized Imidazole-Fused Porphyrin-Donor-Based Dyes: Effect of Linker and Acceptor on Optoelectronic and Photovoltaic Properties. ChemistrySelect, 2018, 3, 2558-2564.	0.7	11
9032	DFT/TD-DFT study on the electronic and spectroscopic properties of hollow cubic and hollow spherical (ZnO) m quantum dots interacting with CO, NO ₂ and SO ₃ molecules. Applied Physics A: Materials Science and Processing, 2018, 124, 1.	1.1	5
9033	The role of inserted polymers in polymeric insulation materials: insights from QM/MD simulations. Journal of Molecular Modeling, 2018, 24, 73.	0.8	1
9034	Molecular structures of metal macrocyclic compounds with nitrogen, oxygen, and sulfur atoms in macrocycles arising in “self-assembly”-processes: quantum-chemical modeling. Structural Chemistry, 2018, 29, 777-802.	1.0	5
9035	Identification of ortho-Substituted Benzoic Acid/Ester Derivatives via the Gas-Phase Neighboring Group Participation Effect in (+)-ESI High Resolution Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2018, 29, 694-703.	1.2	1
9036	Chemi- and Bioluminescence of Cyclic Peroxides. Chemical Reviews, 2018, 118, 6927-6974.	23.0	265
9037	Ab Initio Study of Decay Dynamics of 1-Nitronaphthalene Initiated from the S ₂ (iC* +) Tj ETQq _{1,1} 0.784314 rgBT		
9038	Exploring the Binding of Barbitol to a Synthetic Macrocyclic Receptor. A Charge Density Study. Journal of Physical Chemistry A, 2018, 122, 3031-3044.	1.1	3
9039	Intramolecular stabilization of a catalytic [FeFe]-hydrogenase mimic investigated by experiment and theory. Dalton Transactions, 2018, 47, 4941-4949.	1.6	16
9040	Preparation, characterization, DFT calculations and ethylene oligomerization studies of iron(II) complexes bearing 2-(1H-benzimidazol-2-yl)-phenol derivatives. Journal of Coordination Chemistry, 2018, 71, 1180-1192.	0.8	4
9041	In Depth Analysis of Chiroptical Properties of Enones Derived from Abietic Acid. Journal of Organic Chemistry, 2018, 83, 3547-3561.	1.7	8
9042	A Maze of Dyotropic Rearrangements and Triple Shifts: Carbocation Rearrangements Connecting Stemarene, Stemodene, Betaerdene, Aphidicolene, and Scopadulanol. Journal of Organic Chemistry, 2018, 83, 3780-3793.	1.7	16
9043	A Bit of Sugar on TiO ₂ : Quantum Chemical Insights on the Interfacial Interaction of Glycolaldehyde over Titanium Dioxide. Journal of Physical Chemistry C, 2018, 122, 6041-6051.	1.5	7

#	ARTICLE	IF	CITATIONS
9044	First-Principles Calculations of Point Defects for Quantum Technologies. Annual Review of Materials Research, 2018, 48, 1-26.	4.3	93
9045	Tuning the singlet fission relevant energetic levels of quinoidal bithiophene compounds by means of backbone modifications and functional group introduction. Physical Chemistry Chemical Physics, 2018, 20, 5795-5802.	1.3	8
9046	Tunable Band Gaps of In _x Ga _{1-x} N Alloys: From Bulk to Two-Dimensional Limit. Journal of Physical Chemistry C, 2018, 122, 6930-6942.	1.5	35
9047	Synthesis, characterization, single crystal structure and theoretical studies of trans-Ni(II)-complex with dithiophosphonate ligand. Journal of Molecular Structure, 2018, 1163, 128-136.	1.8	12
9048	Theoretical Study of the Oxidation of Methane to Methanol by the [CuII(CuI(1/4-O)2CuIII(7-N-Etppz))]1+ Complex. Inorganic Chemistry, 2018, 57, 3261-3271.	1.9	9
9049	Multiscale analysis of enantioselectivity in enzyme-catalysed α -keto synthesis using projector-based embedding. Royal Society Open Science, 2018, 5, 171390.	1.1	21
9050	Ultrafast Dynamics of the Metal-to-Ligand Charge Transfer Excited States of Ir(III) Proteo and Deutero Dihydrides. Journal of Physical Chemistry A, 2018, 122, 4430-4436.	1.1	7
9051	Anticorrelated Contributions to Pre-edge Features of Aluminate Near-Edge X-ray Absorption Spectroscopy in Concentrated Electrolytes. Journal of Physical Chemistry Letters, 2018, 9, 2444-2449.	2.1	9
9052	Stereoselective photoredox ring-opening polymerization of O-carboxyanhydrides. Nature Communications, 2018, 9, 1559.	5.8	51
9053	Ultrafast photochemistry of free-base porphyrin: a theoretical investigation of B \rightarrow Q internal conversion mediated by dark states. Physical Chemistry Chemical Physics, 2018, 20, 12483-12492.	1.3	14
9054	Tropospheric Reactions of Triazoles with Hydroxyl Radicals: Hydroxyl Addition is Faster than Hydrogen Abstraction. ChemPhysChem, 2018, 19, 1789-1796.	1.0	3
9055	Random Forest Approach to QSPR Study of Fluorescence Properties Combining Quantum Chemical Descriptors and Solvent Conditions. Journal of Fluorescence, 2018, 28, 695-706.	1.3	16
9056	Non-radiative deactivation of cytosine derivatives at elevated temperature. Molecular Physics, 2018, 116, 2591-2598.	0.8	2
9057	Simplified DFT methods for consistent structures and energies of large systems. Journal of Physics Condensed Matter, 2018, 30, 213001.	0.7	42
9058	Ray-Dutt and Bailar Twists in Fe(II)-Tris(2,2'-bipyridine): Spin States, Sterics, and Fe-N Bond Strengths. Inorganic Chemistry, 2018, 57, 5585-5596.	1.9	25
9059	Effect of the Backbone Tether on the Electrochemical Properties of Soluble Cyclopropenium Redox-Active Polymers. Macromolecules, 2018, 51, 3539-3546.	2.2	43
9060	Understanding Am ³⁺ /Cm ³⁺ separation with H ₄ TPAEN and its hydrophilic derivatives: a quantum chemical study. Physical Chemistry Chemical Physics, 2018, 20, 14031-14039.	1.3	23
9061	Long-range-corrected Rung 3.5 density functional approximations. Journal of Chemical Physics, 2018, 148, 104112.	1.2	18

#	ARTICLE	IF	CITATIONS
9062	Optoelectronics and defect levels in hydroxyapatite by first-principles. <i>Journal of Chemical Physics</i> , 2018, 148, 154706.	1.2	54
9063	Ab initio investigation of the lower-energy candidate structures for (H ₂ O) ₁₀₊ water cluster. <i>Structural Chemistry</i> , 2018, 29, 1273-1285.	1.0	4
9064	Kohn–Sham approach for fast hybrid density functional calculations in real-space numerical grid methods. <i>Computer Physics Communications</i> , 2018, 230, 21-26.	3.0	3
9065	15-Hydroxygermacranolides as Sources of Structural Diversity: Synthesis of Sesquiterpene Lactones by Cyclization and Rearrangement Reactions. Experimental and DFT Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 5480-5495.	1.7	2
9066	Biosynthesis and Conformational Properties of the Irregular Sesquiterpenoids Isothapsadiene and Î²-Isothapsenol. <i>Journal of Organic Chemistry</i> , 2018, 83, 5724-5730.	1.7	2
9067	Kekulé diradicaloids derived from a classical N-heterocyclic carbene. <i>Chemical Science</i> , 2018, 9, 4970-4976.	3.7	55
9068	Molecular dynamics simulations of the structure of mixtures of protic ionic liquids and monovalent and divalent salts at the electrochemical interface. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12767-12776.	1.3	16
9069	Reductive Elimination Leading to C–C Bond Formation in Gold(III) Complexes: A Mechanistic and Computational Study. <i>Chemistry - A European Journal</i> , 2018, 24, 8893-8903.	1.7	28
9070	Ab Initio Methods. , 2018, , 7-197.		2
9071	A highly sensitive pyridine-dicarbohydrazide based chemosensor for colorimetric recognition of Cu ²⁺ , AMP ²⁻ , F ⁻ and AcO ⁻ ions. <i>New Journal of Chemistry</i> , 2018, 42, 8567-8576.	1.4	35
9072	Halogen Photoelimination from Sb ^V Dihalide Corroles. <i>Inorganic Chemistry</i> , 2018, 57, 5333-5342.	1.9	28
9073	Plane-Wave Implementation and Performance of <i>À-la-Carte</i> Coulomb-Attenuated Exchange-Correlation Functionals for Predicting Optical Excitation Energies in Some Notorious Cases. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3184-3195.	2.3	9
9074	Concise total synthesis of (±)-aspidospermidine and computational study: FT-IR, NMR, NBO, NLO, FMO, MEP diagrams. <i>Journal of Molecular Structure</i> , 2018, 1166, 286-303.	1.8	25
9075	Negishi coupling reactions with [¹¹ C]CH ₃ I: a versatile method for efficient ¹¹ C–C bond formation. <i>Chemical Communications</i> , 2018, 54, 4398-4401.	2.2	8
9076	Thermoelectricity in correlated narrow-gap semiconductors. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 183001.	0.7	58
9077	Mechanical Switching of Aromaticity and Homoaromaticity in Molecular Optical Force Sensors for Polymers. <i>Chemistry - A European Journal</i> , 2018, 24, 7340-7344.	1.7	8
9078	Synthesis, Characterization, Solution Behavior, and Density Functional Theory Analysis of Some Pyridinium-Based Ionic Liquids. <i>Journal of Surfactants and Detergents</i> , 2018, 21, 367-373.	1.0	5
9079	A DFT study of structural, electronic and optical properties of heteroatom doped monolayer graphene. <i>Optik</i> , 2018, 168, 228-236.	1.4	15

#	ARTICLE	IF	CITATIONS
9080	Evolution of phosphotriesterase activities of the metallo- β -lactamase family: A theoretical study. <i>Journal of Inorganic Biochemistry</i> , 2018, 184, 8-14.	1.5	9
9081	Electrochemical reduction of carbon dioxide with a molecular polypyridyl nickel complex. <i>Sustainable Energy and Fuels</i> , 2018, 2, 1269-1277.	2.5	19
9082	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2570-2585.	2.3	16
9083	A Description of Enzymatic Catalysis in <i>N</i> -Acetylhexosamine 1-Kinase: Concerted Mechanism of Two-Magnesium-Ion-Assisted GlcNAc Phosphorylation, Flexibility Behavior of Lid Motif upon Substrate Recognition, and Water-Assisted GlcNAc-1-P Release. <i>ACS Catalysis</i> , 2018, 8, 4143-4159.	5.5	19
9084	Molecular Engineering of D π -A-Based Organic Sensitizers for Enhanced Dye-Sensitized Solar Cell Performance. <i>ACS Omega</i> , 2018, 3, 3819-3829.	1.6	32
9085	Combined experimental and theoretical studies on selective sensing of zinc and pyrophosphate ions by rational design of compartmental chemosensor probe: Dual sensing behaviour <i>via</i> secondary recognition approach and cell imaging studies. <i>Dalton Transactions</i> , 2018, 47, 6421-6434.	1.6	31
9086	Cooperative Catalysis with Coupled Chiral Induction in 1,3-Dipolar Cycloadditions of Azomethine Ylides. <i>Chemistry - A European Journal</i> , 2018, 24, 8092-8097.	1.7	12
9087	Development of paper-based chemosensor for the detection of mercury ions using mono- and tetra-sulfur bearing phenanthridines. <i>New Journal of Chemistry</i> , 2018, 42, 8530-8536.	1.4	25
9088	Coumarin/BODIPY Hybridisation for Ratiometric Sensing of Intracellular Polarity Oscillation. <i>Chemistry - A European Journal</i> , 2018, 24, 7513-7524.	1.7	23
9089	Conformational structures and vibrational spectroscopic investigation of isolated dityrosine and tryptophan-tyrosine dipeptides: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2018, 1131, 99-109.	1.1	6
9090	Zwitterionic Rhodium and Iridium Complexes Based on a Carboxylate Bridge-Functionalized Bis-N-heterocyclic Carbene Ligand: Synthesis, Structure, Dynamic Behavior, and Reactivity. <i>Inorganic Chemistry</i> , 2018, 57, 5526-5543.	1.9	17
9091	Self-Interaction Error in Density Functional Theory: An Appraisal. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2353-2358.	2.1	131
9092	Synthesis, DFT study and photoelectrical characterizations of the novel 4-methoxyfuro[3',2':6,7]chromeno[2,3-e]benzo[b][1,4]diazepin-5(12H)-one. <i>Optik</i> , 2018, 166, 294-306.	1.4	21
9093	Piperine derivatives as green corrosion inhibitors on iron surface; DFT, Monte Carlo dynamics study and complexation modes. <i>Journal of Molecular Liquids</i> , 2018, 261, 62-75.	2.3	80
9094	Conformational Plasticity in Tyrosine Kinase Inhibitor-Kinase Interactions Revealed with Fluorescence Spectroscopy and Theoretical Calculations. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4667-4679.	1.2	7
9095	Solvent composition dependent signal reduction of molecular ions generated from aromatic compounds in (+) atmospheric pressure photoionization mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2018, 32, 973-980.	0.7	6
9096	Investigation of carbon monoxide catalytic oxidation on vanadium-embedded graphene. <i>Monatshefte für Chemie</i> , 2018, 149, 1349-1356.	0.9	7
9097	AMOEBAs Polarizable Force Field Parameters of the Heme Cofactor in Its Ferrous and Ferric Forms. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2705-2720.	2.3	5

#	ARTICLE	IF	CITATIONS
9098	A potential method to improve the <i>in vitro</i> cytotoxicity of half-sandwich Os(II) complexes against A2780 cells. Dalton Transactions, 2018, 47, 5714-5724.	1.6	10
9099	Substitution effects in the ¹⁵ N NMR chemical shifts of heterocyclic azines evaluated at the GIAO-DFT level. Magnetic Resonance in Chemistry, 2018, 56, 767-774.	1.1	7
9100	Thermally rearranged polybenzoxazoles made from poly(ortho-hydroxyamide)s. Characterization and evaluation as gas separation membranes. Reactive and Functional Polymers, 2018, 127, 38-47.	2.0	29
9101	A simple and effective solution to the constrained QM/MM simulations. Journal of Chemical Physics, 2018, 148, 134119.	1.2	10
9102	Site-Selective Benzannulation of N-Heterocycles in Bidentate Ligands Leads to Blue-Shifted Emission from [(P^N)Cu] ₂ (X) ₂ Dimers. Inorganic Chemistry, 2018, 57, 4966-4978.	1.9	41
9103	Targeted catalytic degradation of organophosphates: pursuing sensors. Pure and Applied Chemistry, 2018, 90, 1593-1603.	0.9	12
9104	A novel synthesis of octahydropyrido[3,2-]carbazole framework of aspido-spermidine alkaloids and a combined computational, FT-IR, NMR, NBO, NLO, FMO, MEP study of the cis-4a-Ethyl-1-(2-hydroxyethyl)-2,3,4,4a,5,6,7,11c-octahydro-1H-pyrido[3,2-c]carbazole. Journal of Molecular Structure, 2018, 1161, 152-168.	1.8	31
9105	Predicting the Partitioning of Organic Compounds through Polymer Materials: Quantum Mechanical Applications. Journal of Environmental Engineering, ASCE, 2018, 144, .	0.7	3
9106	Carbon dioxide capture by nitrogen containing organic materials – A density functional theory investigation. Computational and Theoretical Chemistry, 2018, 1128, 1-14.	1.1	6
9107	Synthesis, thermodynamic, photophysical and DFT studies of some trivalent metal chelates of a hexadentate tripodal hydroxyquinolate-based ligand. Journal of Coordination Chemistry, 2018, 71, 135-154.	0.8	2
9108	Hydrides, alkalides, and halides of calcium metal chain: electronic structure and NLO property. Structural Chemistry, 2018, 29, 859-870.	1.0	6
9109	Synthesis and properties of the novel (tetraazaporphinato)/(phthalocyaninato) manganese(III) – Pyridyl-substituted [60]fulleropyrrolidine dyads assembled through donor-acceptor bonding. Dyes and Pigments, 2018, 153, 225-232.	2.0	27
9110	How is DMSP decomposed when catalyzed by RIDDP binuclear iron DMSP lyase?. Journal of Catalysis, 2018, 360, 1-8.	3.1	5
9111	Hemisynthesis, computational and molecular docking studies of novel nitrogen containing steroidal aromatase inhibitors: testolactam and testololactam. New Journal of Chemistry, 2018, 42, 4579-4589.	1.4	7
9112	One- and two-dimensional search of an equation of state using a newly released 2DROptimize package. Journal of Physics and Chemistry of Solids, 2018, 116, 131-136.	1.9	3
9113	Investigation on adsorption properties of CO and NO gas molecules on aluminene nanosheet: A density functional application. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2018, 229, 193-200.	1.7	54
9114	Blue luminescent cyanopyridone based molecular architectures: A structure-property study. Journal of Molecular Liquids, 2018, 255, 233-243.	2.3	6
9115	Enantioselective Synthesis of 2,3-Dihydrofurocoumarins by Squaramide-Catalyzed Michael Addition/Cyclization of 4-Hydroxycoumarins with β -Nitrostyrenes. ChemistrySelect, 2018, 3, 1466-1471.	0.7	11

#	ARTICLE	IF	CITATIONS
9116	Thermodynamic, Structural, and Computational Investigation on the Complexation between UO_2^{2+} and Amine-Functionalized Diacetamide Ligands in Aqueous Solution. <i>Inorganic Chemistry</i> , 2018, 57, 2122-2131.	1.9	21
9117	Theoretical Studies on Pd(II)-Catalyzed meta-Selective C-H Bond Arylation of Arenes. <i>ACS Catalysis</i> , 2018, 8, 2498-2507.	5.5	17
9118	Effect of structural manipulation in hetero-tri-aryl amine donor-based $\text{D}\pi\text{A}^2\pi\text{A}$ sensitizers in dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2018, 42, 4361-4371.	1.4	21
9119	Synthesis and characterization of new complexes of nickel (II), palladium (II) and platinum(II) with derived sulfonamide ligand: Structure, DFT study, antibacterial and cytotoxicity activities. <i>Journal of Molecular Structure</i> , 2018, 1161, 345-355.	1.8	90
9120	Unraveling the Role of a Flexible Tetradentate Ligand in the Aerobic Oxidative Carbon-Carbon Bond Formation with Palladium Complexes: A Computational Mechanistic Study. <i>Journal of the American Chemical Society</i> , 2018, 140, 3929-3939.	6.6	12
9121	Penetrating probability and cross section of the Li^+C_{60} encapsulation process through an ab initio molecular dynamics investigation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7007-7013.	1.3	1
9122	Full quantum treatment of charge dynamics in amorphous molecular semiconductors. <i>Physical Review B</i> , 2018, 97, .	1.1	31
9123	Synthesis, characterization and computational investigation of novel metalloporphyrazines containing 15-membered O2S2-donor macrocyclic moieties. <i>Journal of Porphyrins and Phthalocyanines</i> , 2018, 22, 207-220.	0.4	2
9124	Adsorption behavior of NH_3 and NO_2 molecules on stanene and stanane nanosheets: A density functional theory study. <i>Chemical Physics Letters</i> , 2018, 695, 162-169.	1.2	50
9125	Spectroscopic and Structural Characterization of Mn(III)-Alkylperoxo Complexes Supported by Pentadentate Amide-Containing Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 2489-2502.	1.9	17
9126	Theoretical Study and Experimental Analysis on 2-(1-Ethyl-4-hydroxy-2-oxo-1,2-dihydroquinolin-3-yl)-2-oxoacetic Acid (3) Using the DFT Approach. <i>Journal of Solution Chemistry</i> , 2018, 47, 172-197.	0.6	1
9127	Understanding the reaction mechanism of the oxidative addition of ammonia by $(\text{PXP})\text{Ir}(\text{scp})$ complexes: the role of the X group. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1105-1113.	1.3	18
9128	An Air-Stable Molybdenum-Based Precatalyst in Oxygen-Atom Transfer Reactions. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 1427-1434.	1.0	3
9129	Dithienopicenocarbazole-Based Acceptors for Efficient Organic Solar Cells with Optoelectronic Response Over 1000 nm and an Extremely Low Energy Loss. <i>Journal of the American Chemical Society</i> , 2018, 140, 2054-2057.	6.6	369
9130	Supersaturated calcium carbonate solutions are classical. <i>Science Advances</i> , 2018, 4, eaao6283.	4.7	116
9131	Comparison of Interfacial Electron Transfer Efficiency in $[\text{Fe}(\text{ctpy})_2]^{2+}$ and $[\text{Fe}(\text{cCNC})_2]^{2+}$ TiO_2 Assemblies: Importance of Conformational Sampling. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1821-1830.	1.1	9
9132	Electrocatalytic Reduction of CO_2 to Formate by an Iron Schiff Base Complex. <i>Inorganic Chemistry</i> , 2018, 57, 2111-2121.	1.9	97
9133	Conflict in the Mechanism and Kinetics of the Barrierless Reaction between SH and NO_2 Radicals. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1926-1937.	1.1	7

#	ARTICLE	IF	CITATIONS
9134	Electron-phonon coupling from finite differences. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 083001.	0.7	58
9135	A Perylene-Triazine-Based Star-Shaped Green Light Emitter for Organic Light Emitting Diodes. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 1608-1613.	1.2	30
9136	Heparin and Heparan Sulfate Binding of the Antiparasitic Drug Imidocarb: Circular Dichroism Spectroscopy, Isothermal Titration Calorimetry, and Computational Studies. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1781-1791.	1.2	15
9137	Multiscale modeling of enzymes: QM-cluster, QM/MM, and QM/MM/MD: A tutorial review. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25558.	1.0	106
9138	Excited-State Processes of Cyclometalated Platinum(II) Charge-Transfer Dimers Bridged by Hydroxypyridines. <i>Inorganic Chemistry</i> , 2018, 57, 1298-1310.	1.9	43
9139	Reaction of Pentanol isomers with OH radical—A theoretical perspective. <i>Molecular Physics</i> , 2018, 116, 1153-1165.	0.8	8
9140	A chiral lactate reporter based on total and circularly polarized Tb(III) luminescence. <i>New Journal of Chemistry</i> , 2018, 42, 7931-7939.	1.4	33
9141	The Nature of the Technetium Species Formed During the Oxidation of Technetium Dioxide with Oxygen and Water. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 1137-1144.	1.0	8
9142	Ultrasonic and bio-assisted synthesis of Ag@HNTs as a novel heterogeneous catalyst for the green synthesis of propargylamines: A combination of experimental and computational study. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4291.	1.7	30
9143	Three-Component Activation/Alkynylation/Cyclocondensation (AACC) Synthesis of Enhanced Emission Solvatochromic β -Ethynylquinoxalines. <i>Chemistry - A European Journal</i> , 2018, 24, 8114-8125.	1.7	22
9144	Synthesis and Characterization of an Osmapentalene Derivative Containing a η^2 -Agostic Os-Ag-H-C(sp ³) Interaction. <i>Organometallics</i> , 2018, 37, 618-623.	1.1	12
9145	Electronic structure calculations and nonadiabatic dynamics simulations of excited-state relaxation of Pigment Yellow 101. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6524-6532.	1.3	9
9146	Stimuli responsive AIE active positional isomers of phenanthroimidazole as non-doped emitters in OLEDs. <i>Journal of Materials Chemistry C</i> , 2018, 6, 2077-2087.	2.7	95
9147	Near-UV Water Splitting by Cu, Ni, and Co Complexes in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2069-2078.	1.1	3
9148	Comparison of measured and predicted specific optical rotation in gas and solution phases: A test for the polarizable continuum model of solvation. <i>Chirality</i> , 2018, 30, 383-395.	1.3	17
9149	Reactivity of hydropersulfides toward the hydroxyl radical unraveled: disulfide bond cleavage, hydrogen atom transfer, and proton-coupled electron transfer. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4793-4804.	1.3	9
9150	Designing of Efficient Acceptors for Organic Solar Cells: Molecular Modelling at DFT Level. <i>Journal of Cluster Science</i> , 2018, 29, 359-365.	1.7	46
9151	Spontaneous Isomerization of Peptide Cation Radicals Following Electron Transfer Dissociation Revealed by UV-Vis Photodissociation Action Spectroscopy. <i>Journal of the American Society for Mass Spectrometry</i> , 2018, 29, 1768-1780.	1.2	4

#	ARTICLE	IF	CITATIONS
9152	Novel Bonding Mode in Phosphine Haloboranes. ACS Omega, 2018, 3, 608-614.	1.6	3
9153	Morphology of Anion-Conducting Ionenes Investigated by X-ray Scattering and Simulation. Journal of Physical Chemistry B, 2018, 122, 1730-1737.	1.2	13
9154	Exciton Localization on Ru-Based Photosensitizers Induced by Binding to Lipid Membranes. Journal of Physical Chemistry Letters, 2018, 9, 683-688.	2.1	14
9155	Establishment of Molecular Design Strategy To Obtain Activatable Fluorescent Probes for Carboxypeptidases. Journal of the American Chemical Society, 2018, 140, 1767-1773.	6.6	55
9156	Mechanistic insights into the tropo-inversion of the biphenyl moiety in chiral bis-amido phosphites and in their palladium(ii) complexes. Dalton Transactions, 2018, 47, 2292-2305.	1.6	5
9157	Electronic versus steric effects of pyridinophane ligands on Pd(III) complexes. Dalton Transactions, 2018, 47, 1151-1158.	1.6	13
9158	Structural and quantum mechanical computations to elucidate the altered binding mechanism of metal and drug with pyrazinamidase from Mycobacterium tuberculosis due to mutagenicity. Journal of Molecular Graphics and Modelling, 2018, 80, 126-131.	1.3	15
9159	Inheritance of Photochromic Properties of Nitro-Substituted and Halogenated Spiropyrans Containing the Pyrrolidino[60]fullerene. Journal of Physical Chemistry A, 2018, 122, 505-515.	1.1	13
9160	Built-In Potentials Induced by Molecular Order in Amorphous Organic Thin Films. ACS Applied Materials & Interfaces, 2018, 10, 1881-1887.	4.0	59
9161	Insights into Molecular Structures and Optical Properties of Stacked [Au ₃ (RN-CR ²) ₃] _n Complexes. Inorganic Chemistry, 2018, 57, 718-730.	1.9	13
9162	Exploring the relevance of thiophene rings as bridge unit in acceptor-bridge-donor dyes on self-aggregation and performance in DSSCs. Journal of Computational Chemistry, 2018, 39, 685-698.	1.5	10
9163	Synthesis, spectroscopic and DFT studies of novel 4-(morpholinomethyl)-5-oxo-1-phenylpyrrolidine-3-carboxylic acid. Journal of Molecular Structure, 2018, 1157, 551-559.	1.8	7
9164	The influence of the double-ring nanotubules diameter of Bn (n=14, 20, 24 and 32) on the electronic and structural properties due to lithium atom doping: quantum chemistry approach. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	0
9165	Synthesis and Photochemical Properties of 2,3,5,6-bis(cyclohexano)-BODIPY. Journal of Fluorescence, 2018, 28, 393-407.	1.3	6
9166	Mechanism and kinetics for the reaction of fulminic acid, HCNO, with an amino radical, NH ₂ . Combustion and Flame, 2018, 190, 317-326.	2.8	3
9167	Molecular modeling for the investigation of UV absorbers for sunscreens: Triazine and benzotriazole derivatives. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 356, 219-229.	2.0	22
9168	Experimental Evidence for Noncanonical Thymine Cation Radicals in the Gas Phase. Journal of Physical Chemistry B, 2018, 122, 86-97.	1.2	18
9169	Unraveling the Critical Role Played by Ado ⁷⁶ 2-OH in the Post-Transfer Editing by Archaeal Threonyl-tRNA Synthetase. Journal of Physical Chemistry B, 2018, 122, 1092-1101.	1.2	10

#	ARTICLE	IF	CITATIONS
9170	Benzopyrano-fused N-heterocyclic Polyaromatics. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 532-536.	1.2	14
9171	Are beryllium-containing biphenyl derivatives efficient anion sponges?. <i>Journal of Molecular Modeling</i> , 2018, 24, 16.	0.8	7
9172	The Bethe-Salpeter equation in chemistry: relations with TD-DFT, applications and challenges. <i>Chemical Society Reviews</i> , 2018, 47, 1022-1043.	18.7	158
9173	Investigating the interaction of aminopolycarboxylic acid (APCA) ligands with silver nanoparticles: A Raman, surface-enhanced Raman and density functional theoretical study. <i>Journal of Molecular Structure</i> , 2018, 1156, 592-601.	1.8	9
9174	Rational Density Functional Selection Using Game Theory. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 61-67.	2.5	20
9175	Kinetics of the Strain-Promoted Oxidation-Controlled Cycloalkyne-1,2-quinone Cycloaddition: Experimental and Theoretical Studies. <i>Journal of Organic Chemistry</i> , 2018, 83, 244-252.	1.7	24
9176	Conformational analysis of some 4-substituted 2-(phenylselanyl)-2-(methoxy)-acetophenones. <i>Journal of Molecular Structure</i> , 2018, 1157, 29-39.	1.8	3
9177	Mechanistic Aspects of Acrylic Acid Formation from CO ₂ Ethylene Coupling over Palladium- and Nickel-based Catalysts. <i>ChemCatChem</i> , 2018, 10, 1420-1430.	1.8	20
9178	Coupled Electrocyclization/Prototropic Shift in the Biosynthesis of Crotoninsolidane Diterpenoids. <i>Journal of Organic Chemistry</i> , 2018, 83, 1073-1076.	1.7	4
9179	Mechanism and <i>cis/trans</i> Selectivity of Vinylogous Nazarov-type [6π] Photocyclizations. <i>Journal of Organic Chemistry</i> , 2018, 83, 964-972.	1.7	16
9180	Preparation of multiblock copolymers <i>via</i> step-wise addition of <i>l</i> -lactide and trimethylene carbonate. <i>Chemical Science</i> , 2018, 9, 2168-2178.	3.7	28
9181	Conformers, properties, and docking mechanism of the anticancer drug docetaxel: DFT and molecular dynamics studies. <i>Journal of Computational Chemistry</i> , 2018, 39, 889-900.	1.5	10
9182	A Dihydrodinaphthoheptacene. <i>Journal of Organic Chemistry</i> , 2018, 83, 1891-1897.	1.7	9
9183	Unexpected cleavage of upper rim-bridged calix[4]arenes leading to linear oligophenolic derivatives. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 838-843.	1.5	6
9184	How are the charge transfer descriptors affected by the quality of the underpinning electronic density?. <i>Journal of Computational Chemistry</i> , 2018, 39, 735-742.	1.5	22
9185	Homogeneously Catalyzed Electroreduction of Carbon Dioxide—Methods, Mechanisms, and Catalysts. <i>Chemical Reviews</i> , 2018, 118, 4631-4701.	23.0	858
9186	How do London Dispersion Interactions Impact the Photochemical Processes of Molecular Switches?. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 464-470.	2.1	22
9187	Catalytic effect of a single water molecule on the OH + CH ₂ NH reaction. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4297-4307.	1.3	35

#	ARTICLE	IF	CITATIONS
9188	Activation of H ₂ by Gadolinium Cation (Gd ⁺): Bond Energy of GdH ⁺ and Mechanistic Insights from Guided Ion Beam and Theoretical Studies. <i>Journal of Physical Chemistry A</i> , 2018, 122, 750-761.	1.1	8
9189	Ground state geometries, UV/vis absorption spectra and charge transfer properties of triphenylamine-thiophenes based dyes for DSSCs: A TD-DFT benchmark study. <i>Computational and Theoretical Chemistry</i> , 2018, 1125, 39-48.	1.1	56
9190	Computational Assessment of Relative Sites Stabilities and Site-Specific Adsorptive Properties of Titanium Silicalite-1. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1612-1621.	1.5	18
9191	6-Shaped Benzimidazole Derivatives as Blue-Emitting Materials: The Role of C2 Substituents on Photophysical Properties. <i>Asian Journal of Organic Chemistry</i> , 2018, 7, 729-738.	1.3	4
9192	Benchmark-Quality Semiexperimental Structural Parameters of van der Waals Complexes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1077-1087.	1.1	16
9193	Pentacoordinated Rhodium(I) Complexes Supported by Coumarin-Functionalized <i>N</i> -Heterocyclic Carbene Ligands. <i>Organometallics</i> , 2018, 37, 191-202.	1.1	26
9194	New di-anchoring A-D-A configured organic chromophores for DSSC application: sensitization and co-sensitization studies. <i>Photochemical and Photobiological Sciences</i> , 2018, 17, 302-314.	1.6	47
9195	Valence bonds in elongated boron clusters. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25575.	1.0	8
9196	Sucrose capped gold nanoparticles as a plasmonic chemical sensor based on non-covalent interactions: Application for selective detection of vitamins B1 and B6 in brown and white rice food samples. <i>Food Chemistry</i> , 2018, 250, 14-21.	4.2	42
9197	How Does the Catalyst Affect the Reaction Pathway? DFT Analysis of the Mechanism and Selectivity in the 1,6-Diyne Ester Cycloisomerization. <i>Organometallics</i> , 2018, 37, 261-270.	1.1	8
9198	Palladium/Norbornene-Catalyzed <i>ortho</i> Aliphatic Acylation with Mixed Anhydride: Selectivity and Reactivity. <i>Organic Letters</i> , 2018, 20, 325-328.	2.4	30
9199	Electronic, nonlinear optical and thermodynamic properties of (CdS) <i>n</i> clusters: A first principle study. <i>Computational Condensed Matter</i> , 2018, 14, 40-45.	0.9	12
9200	Photophysics and peripheral ring size dependent aggregate emission of cross-conjugated enediynes: applications to white light emission and vapor sensing. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4167-4180.	1.3	7
9201	Overview of Computational Methods for Organic Chemists. , 2018, , 31-67.		3
9202	Microwave-Assisted Expedited Green Synthesis, Photophysical, Computational Studies of Coumarin-3-acyl-thiazol-4-ylidene-2,4-thiazolin-3-ones and Their Anticancer Activity. <i>ChemistrySelect</i> , 2018, 3, 4448-4462.	0.8	21
9203	Alternative mechanisms of thermal decomposition of <i>o</i> -nitrotoluene in the gas phase. <i>Russian Chemical Bulletin</i> , 2018, 67, 274-281.	0.4	4
9204	Diversity-oriented four-component synthesis of solid state luminescent difluoro oxazaborinines. <i>Dyes and Pigments</i> , 2018, 157, 198-217.	2.0	10
9205	Energies of selected conformers/rotamers of the unsubstituted linear polyenes C _{2n} H _{2n+2} : Results at the B3LYP/6-311++G(d,p) (n = 14) and MP2(FC)/aug-cc-pVDZ (n = 7) computational levels. <i>Chemical Data Collections</i> , 2018, 15-16, 97-106.		

#	ARTICLE	IF	CITATIONS
9206	A combined density functional theory and numerical simulation investigation of levels of chirality transfer and regioselectivity for the radical cyclizations of <i>N</i> -methyl-, <i>N</i> -ethyl- and <i>N</i> -isopropyl-substituted <i>ortho</i> -halo- <i>N</i> -acryloylanilides. <i>New Journal of Chemistry</i> , 2018, 42, 9783-9790.	1.4	1
9207	Electronic structure, magnetism, and exchange integrals in transition-metal oxides: Role of the spin polarization of the functional in DFT+ U calculations. <i>Physical Review B</i> , 2018, 97, .	1.1	20
9208	Influence of the Metal Ion on the Electrocatalytic Hydrogen Production by a Thiosemicarbazone Palladium Complex. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 2259-2266.	1.0	23
9209	Carbon dioxide capture using covalent organic frameworks (COFs) type material—a theoretical investigation. <i>Journal of Molecular Modeling</i> , 2018, 24, 120.	0.8	12
9210	Anion effect on the conformational equilibrium of sulfamide and its <i>N,N</i> -diindolyl derivative: Insights on anion transportation. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3850.	0.9	1
9211	Computational study on night-time reaction of 1, 1-Dichlorodimethylether (DCDME) CH ₃ OCHCl ₂ with NO ₃ radical and the fortuity of alkoxy radical CH ₃ OC(O)Cl ₂ . <i>Chemical Physics Letters</i> , 2018, 701, 157-164.	1.2	5
9212	Improvement of photovoltaic performances by optimizing π -conjugated bridge for the C217-based dyes: A theoretical perspective. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 360, 137-144.	2.0	2
9213	Transition metal hydrides MH_{n+1}^{\ominus} ($M = Sc \sim Zn$): Benchmark study and periodic trends. <i>Computational and Theoretical Chemistry</i> , 2018, 1134, 15-21.	1.1	2
9214	Theoretical investigation of $M@Pb_{12}^{2+}$ and $M@Sn_{12}^{2+}$ Zintl clusters ($M = Lr_{n+1}, Lu_n$, Tj ETQqO O 0 rgBJ, Overlock 10 Tf 50		
9215	Assessment of interaction-strength interpolation formulas for gold and silver clusters. <i>Journal of Chemical Physics</i> , 2018, 148, 134106.	1.2	28
9216	Diselenoamino acid derivatives as GPx mimics and as substrates of TrxR: in vitro and in silico studies. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 3777-3787.	1.5	22
9217	Optical properties of body-centered tetragonal C4: Insights from many-body perturbation and time-dependent density functional theories. <i>Journal of Applied Physics</i> , 2018, 123, 165107.	1.1	0
9218	The anti-epileptic drug lamotrigine inhibits the CYP17A1 lyase reaction in vitro. <i>Biology of Reproduction</i> , 2018, 99, 888-897.	1.2	3
9219	Computational investigations of click-derived 1,2,3-triazoles as keystone ligands for complexation with transition metals: a review. <i>RSC Advances</i> , 2018, 8, 12232-12259.	1.7	33
9220	Efficient near-infrared emission of π -extended cyclometalated iridium complexes based on pyrene in solution-processed polymer light-emitting diode. <i>Chemical Physics Letters</i> , 2018, 699, 99-106.	1.2	23
9221	Density functional theory calculations of the water interactions with ZrO ₂ nanoparticles Y ₂ O ₃ doped. <i>Journal of Physics: Conference Series</i> , 2018, 994, 012013.	0.3	11
9222	Comparison of atmospheric reactions of NH ₃ and NH ₂ with hydroxyl radical on the singlet, doublet and triplet potential energy surfaces, kinetic and mechanistic study. <i>Chemical Physics</i> , 2018, 507, 51-69.	0.9	8
9223	Theoretical design of new small molecules with a low band-gap for organic solar cell applications: DFT and TD-DFT study. <i>Computational Materials Science</i> , 2018, 150, 54-61.	1.4	41

#	ARTICLE	IF	CITATIONS
9224	Gold(<i>ortho</i> -(alkynyl) styrenes: DFT analysis of the crucial role of SbF ₆ ⁻ in the elimination of protons. <i>Catalysis Science and Technology</i> , 2018, 8, 2441-2448.	2.1	18
9225	Bay Annulated Indigo as a New Chromophore for π -Type Dye-Sensitized Solar Cells. <i>ChemPhotoChem</i> , 2018, 2, 498-506.	1.5	12
9226	Nickel-Alkyl Complexes with a Reactive PNC-Pincer Ligand. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 2408-2418.	1.0	20
9227	Influence of the protein and DFT method on the broken symmetry and spin states in nitrogenase. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25627.	1.0	42
9228	Predicting Optical Properties from Ab Initio Calculations. <i>Springer Series in Surface Sciences</i> , 2018, , 83-104.	0.3	0
9229	First principle investigation of the mechanical properties of natural layered nanocomposite: Clinocllore as a model system for heterodesmic structures. <i>Composite Structures</i> , 2018, 202, 551-558.	3.1	22
9230	Synthesis, Characterization and Performance Studies of a New Metal-Free Organic Sensitizer for DSSC application. <i>Materials Today: Proceedings</i> , 2018, 5, 3150-3157.	0.9	12
9231	Dual-Level Approach to Instanton Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1865-1872.	2.3	18
9232	Theoretical study of native point defects in strained-layer superlattice systems. <i>Journal of Applied Physics</i> , 2018, 123, 161414.	1.1	5
9233	Stabilising fleeting intermediates of stilbene photocyclization with amino-borane functionalisation: the rare isolation of persistent dihydrophenanthrenes and their [1,5] H-shift isomers. <i>Chemical Science</i> , 2018, 9, 3844-3855.	3.7	32
9234	Reversible modulation of the redox characteristics of acid-sensitive molybdenum and tungsten scorpionate complexes. <i>Dalton Transactions</i> , 2018, 47, 6323-6332.	1.6	10
9235	Theoretical screening and design of SM315-based porphyrin dyes for highly efficient dye-sensitized solar cells with near-IR light harvesting. <i>Dyes and Pigments</i> , 2018, 155, 292-299.	2.0	41
9236	Quantum chemical study on the reaction mechanism and kinetics of Cl-initiated oxidation of methyl n-propyl ether. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	4
9237	Short-range density functional correlation within the restricted active space CI method. <i>Journal of Chemical Physics</i> , 2018, 148, 124118.	1.2	17
9238	Mechanistic study of the [(dpp-bian)Re(CO) ₃ Br] electrochemical reduction using in situ EPR spectroscopy and computational chemistry. <i>Electrochimica Acta</i> , 2018, 270, 526-534.	2.6	21
9239	Analysis of polarization in hydrogen bonded complexes: An asymptotic projection approach. <i>Chemical Physics Letters</i> , 2018, 696, 1-7.	1.2	0
9240	Dataset on the piezo-spectroscopic behaviour of hydroxylapatite: Effect of mechanical stress on the Raman and Infrared vibrational bands from ab initio quantum mechanical simulations. <i>Data in Brief</i> , 2018, 18, 325-333.	0.5	3
9241	Spectroscopy in Complex Environments from QM-MM Simulations. <i>Chemical Reviews</i> , 2018, 118, 4071-4113.	23.0	136

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9242	Analysis of the structures, energetics, and vibrational frequencies for the hydrogen-bonded interaction of nucleic acid bases with Carmustine pharmaceutical agent: a detailed computational approach. <i>Structural Chemistry</i> , 2018, 29, 1165-1174.	1.0	11
9243	An accurate first-principles treatment of doping-dependent electronic structure of high-temperature cuprate superconductors. <i>Communications Physics</i> , 2018, 1, .	2.0	94
9244	Spin-Orbit Splittings and Low-Lying Electronic States of AuSi and AuGe: Anion Photoelectron Spectroscopy and <i>ab Initio</i> Calculations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3374-3382.	1.1	13
9245	Investigation on the performance of PCM/TD-DFT functionals (standard pure, hybrid and long-range) Tj ETQq1 1 0.784314 rgBT /Over 1-(2,5-dimethylfuran-3-yl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one dye in different solvents. <i>Journal of Molecular Structure</i> , 2018, 1164, 289-296.	1.8	6
9246	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2596-2608.	2.3	202
9247	Modeling L _{2,3} -Edge X-ray Absorption Spectroscopy with Real-Time Exact Two-Component Relativistic Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1998-2006.	2.3	44
9248	A theoretical study of UV-Vis spectrum and antioxidant activity of chryso-obtusin. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1850015.	1.8	0
9249	QM/MM study of the reaction mechanism of sulfite oxidase. <i>Scientific Reports</i> , 2018, 8, 4684.	1.6	22
9250	Multiorientation Model for Planar Ordering of Trimesic Acid Molecules. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7344-7352.	1.5	19
9251	Theoretical Investigation on Ni-Catalyzed C(sp ³)-F Activation and Ring Contraction of Tetrahydropyrans: Exploration of an SN ₂ Pathway. <i>Organometallics</i> , 2018, 37, 1114-1122.	1.1	8
9252	<i>para</i> -Aminosalicylic acid in the treatment of manganese toxicity. Complexation of Mn ²⁺ with 4-amino-2-hydroxybenzoic acid and its <i>N</i> -acetylated metabolite. <i>New Journal of Chemistry</i> , 2018, 42, 8035-8049.	1.4	14
9253	An Unprecedented Retro-Mumm Rearrangement Revealed by ES-MS/MS, IRMPD Spectroscopy, and DFT Calculations. <i>Chemistry - A European Journal</i> , 2018, 24, 7026-7032.	1.7	14
9254	Theoretical prediction of the mechanistic pathways and kinetics of methylcyclohexane initiated by OH radicals. <i>Molecular Physics</i> , 2018, 116, 1589-1597.	0.8	1
9255	Magnetically Induced Ring-Current Strengths in Möbius Twisted Annulenes. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1627-1632.	2.1	19
9256	An efficient and weak efficiency-roll-off near-infrared (NIR) polymer light-emitting diode (PLED) based on a PVK-supported Zn ²⁺ -Yb ³⁺ -containing metallopolymer. <i>Journal of Materials Chemistry C</i> , 2018, 6, 4114-4121.	2.7	23
9257	Elucidation of the anticancer potential and tubulin isotype-specific interactions of Î ² -sitosterol. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 195-208.	2.0	20
9258	Hydrogen atom transfer in metal ion complexes of the glutathione thyl radical. <i>International Journal of Mass Spectrometry</i> , 2018, 429, 39-46.	0.7	5
9259	Electronic structures and photophysical properties of phosphorescent platinum (II) complexes with tridentate C ^N *N cyclometalated ligands. <i>Applied Organometallic Chemistry</i> , 2018, 32, e3929.	1.7	8

#	ARTICLE	IF	CITATIONS
9260	Quantum mechanical and spectroscopic (FT-IR, FT-Raman) study, NBO analysis, HOMO-LUMO, first order hyperpolarizability and molecular docking study of methyl[(3R)-3-(2-methylphenoxy)-3-phenylpropyl]amine by density functional method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 188, 382-393.	2.0	57
9261	ELSI: A unified software interface for Kohn-Sham electronic structure solvers. <i>Computer Physics Communications</i> , 2018, 222, 267-285.	3.0	78
9262	Stereoselective reduction of the bioactive 19-nor-clerodane trans-dehydrocrotonin by using sodium borohydride and cerium (III) chloride as a catalyst. <i>Journal of Molecular Structure</i> , 2018, 1154, 626-635.	1.8	2
9263	1,4-Naphthoquinones potently inhibiting P2X7 receptor activity. <i>European Journal of Medicinal Chemistry</i> , 2018, 143, 1361-1372.	2.6	31
9264	Cd(II) and Ni(II) complexes from aroyl hydrazones: Unravelling the intermolecular interactions and electronic, crystal structures through experimental and theoretical studies. <i>Inorganica Chimica Acta</i> , 2018, 469, 264-279.	1.2	23
9265	Conformational behavior, redox and spectroscopic properties of gold dithiolene complexes: [Au(iPr-thiazYdt) ₂] ⁺¹ (Y = O, S, Se). <i>Inorganica Chimica Acta</i> , 2018, 469, 255-263.	1.2	3
9266	<sc>DFT</sc> study of the acid-catalyzed esterification reaction mechanism of methanol with carboxylic acid and its halide derivatives. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25497.	1.0	41
9267	Fluorescent pyridopyrimidine fused pyranones - design, synthesis, fluorescent whitening and DFT studies. <i>Journal of Luminescence</i> , 2018, 194, 248-256.	1.5	12
9268	Workflows and performances in the ranking prediction of 2016 D3R Grand Challenge 2: lessons learned from a collaborative effort. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 129-142.	1.3	8
9269	One-dimensional diamondoid polyaniline-like nanothreads from compressed crystal aniline. <i>Chemical Science</i> , 2018, 9, 254-260.	3.7	66
9270	Oxygen bridged Homobinuclear Mn(II) compounds with Anthranilic acid: Theoretical calculations, oxidation and catalase activity. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4105.	1.7	5
9271	Structural and Electronic Properties of Defect-Free and Defect-Containing Polypropylene: A Computational Study by van der Waals Density-Functional Method. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1700036.	0.7	4
9272	Tuning the locus of oxidation in Cu-diamido-diphenoxo complexes: From Cu(III) to Cu(II)-phenoxyl radical. <i>Inorganica Chimica Acta</i> , 2018, 481, 143-150.	1.2	7
9273	Experimental and theoretical analysis of a rare nitrate bridged 3d-4f complex containing LaZn ₂ core synthesized from a Zn(II) metalloligand. <i>Journal of Molecular Structure</i> , 2018, 1153, 85-95.	1.8	8
9274	Synthesis, molecular, electronic structure, linear and non-linear optical and phototransient properties of 8-methyl-1,2-dihydro-4H-chromeno[2,3-b]quinoline-4,6(3H)-dione (MDCQD): Experimental and DFT investigations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 478-490.	2.0	29
9275	Synthesis and characterization of Ni(II) complexes bearing of 2-(1H-benzimidazol-2-yl)phenol derivatives as highly active catalysts for ethylene oligomerization. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4015.	1.7	15
9276	Incorporating quinoxaline unit as additional acceptor for constructing efficient donor-free solar cell sensitizers. <i>Dyes and Pigments</i> , 2018, 149, 65-72.	2.0	10
9277	Excited-state proton transfer induced [4 + 2] and [4 + 4] photocycloaddition reactions of an oxazoline: Mechanism and selectivity. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 355, 256-266.	2.0	4

#	ARTICLE	IF	CITATIONS
9278	Kinetics and mechanistic study of polynuclear platinum(II) polypyridyl complexes; A paradigm shift in search of new anticancer agents. <i>Inorganica Chimica Acta</i> , 2018, 469, 341-352.	1.2	8
9279	Preparation of a coordinatively saturated $\lambda^4\text{-}\lambda^2\text{-}\lambda^2$ -peroxodicopper(II) compound. <i>Inorganica Chimica Acta</i> , 2018, 481, 166-170.	1.2	4
9280	Solvatochromic isocyanonaphthalene dyes as ligands for silver(I) complexes, their applicability in silver(I) detection and background reduction in biolabelling. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 2555-2567.	4.0	12
9281	Structural, luminescence, thermodynamic and theoretical studies on mononuclear complexes of Eu(III) with pyridine monocarboxylate-N-oxides in aqueous solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 150-163.	2.0	12
9282	Equatorial coordination of uranyl: Correlating ligand charge donation with the Oyl-U-Oyl asymmetric stretch frequency. <i>Journal of Organometallic Chemistry</i> , 2018, 857, 94-100.	0.8	6
9283	Structure and function of a novel antioxidant peptide from the skin of tropical frogs. <i>Free Radical Biology and Medicine</i> , 2018, 115, 68-79.	1.3	52
9284	A computational study of photonic materials based on Ni bis(dithiolene) fused with benzene, possessing gigantic second hyperpolarizabilities. <i>Journal of Materials Chemistry C</i> , 2018, 6, 91-110.	2.7	14
9285	Computational and <i>in vitro</i> insights on snake venom phospholipase A ₂ inhibitor of phytocompound <i>ikshusterol-3-O-glucoside</i> of <i>Clematis gouriana</i> Roxb. ex DC.. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 4197-4208.	2.0	10
9286	Acid-triggered O ² O Bond Heterolysis of a Nonheme Fe ^{III} (OOH) Species for the Stereospecific Hydroxylation of Strong C-H Bonds. <i>Chemistry - A European Journal</i> , 2018, 24, 5331-5340.	1.7	43
9287	Revealing the Unique Properties of Platinum(II) Complexes with Bidentate Bis(o-carborane) Ligands. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 99-108.	1.0	6
9288	Porphyrin-Based Air-Stable Helical Radicals. <i>Chemistry - A European Journal</i> , 2018, 24, 572-575.	1.7	52
9289	Quantum mechanical, spectroscopic study (FT-IR and FT-Raman), NBO analysis, HOMO-LUMO, first order hyperpolarizability and docking studies of a non-steroidal anti-inflammatory compound. <i>Journal of Molecular Structure</i> , 2018, 1156, 645-656.	1.8	75
9290	Extension of the Polarizable Charge Equilibration Model to Higher Oxidation States with Applications to Ge, As, Se, Br, Sn, Sb, Te, I, Pb, Bi, Po, and At Elements. <i>Journal of Physical Chemistry A</i> , 2018, 122, 639-645.	1.1	14
9291	Mapping the 3D orientation of piconewton integrin traction forces. <i>Nature Methods</i> , 2018, 15, 115-118.	9.0	105
9292	How accurate is the description of ligand-protein interactions by a hybrid QM/MM approach?. <i>Journal of Molecular Modeling</i> , 2018, 24, 11.	0.8	19
9293	On lithium doping in two stable nano-flakes of the B24: The double-ring versus the quasiplanar configuration. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 79, 213-222.	1.3	0
9294	Novel nonequilibrium solvation theory for calculating the vertical ionization energies of alkali metal cations and DNA bases in aqueous. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	2
9295	Diffuse electron of alkali metals (Li, Na, K) or diffuse electron pair of alkaline earth metals (Be, Mg.) <i>Tj ETQq1 1 0.784314 rgBT /Overlook</i> compounds. <i>Chemical Physics Letters</i> , 2018, 692, 160-165.	1.2	8

#	ARTICLE	IF	CITATIONS
9296	Theoretical calculations of homogeneous catalysis in the gas phase: elimination kinetics of 2,2-dimethoxypropane in the presence of HCl, F_3CCOOH and CH_3COOH . <i>Molecular Physics</i> , 2018, 116, 1118-1126.	0.8	3
9297	Corrected Polarizable Embedding: Improving the Induction Contribution to Perichromism for Linear Response Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 833-842.	2.3	12
9298	Theoretical Study on the Photoinduced Electron Transfer Mechanisms of Different Peroxynitrite Probes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 217-223.	1.1	8
9299	First-principles study of intrinsic defects in CdO. <i>International Journal of Modern Physics B</i> , 2018, 32, 1850059.	1.0	17
9300	Organocatalytic Enantioselective Higher-Order Cycloadditions of In Situ Generated Amino Isobenzofulvenes. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 1246-1250.	7.2	42
9301	The bridged effect on the geometric, optoelectronic and charge transfer properties of the triphenylamine-bithiophene-based dyes: a DFT study. <i>Research on Chemical Intermediates</i> , 2018, 44, 2009-2023.	1.3	32
9302	Highly Electrophilic, Catalytically Active and Redox-Responsive Cobaltoceniumyl and Ferrocenyl Triazolylidene Coinage Metal Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 3742-3753.	1.7	67
9303	N-doped cycloparaphenylenes: Tuning electronic properties for applications in thermally activated delayed fluorescence. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25562.	1.0	9
9304	Electrocatalytic Reduction of Dioxygen to Hydrogen Peroxide by a Molecular Manganese Complex with a Bipyridine-Containing Schiff Base Ligand. <i>Journal of the American Chemical Society</i> , 2018, 140, 3232-3241.	6.6	56
9305	Band-like Charge Photogeneration at a Crystalline Organic Donor/Acceptor Interface. <i>Advanced Energy Materials</i> , 2018, 8, 1701494.	10.2	23
9306	Roadmap on semiconductor-cell biointerfaces. <i>Physical Biology</i> , 2018, 15, 031002.	0.8	45
9307	First-principles investigation on structural and electronic properties of antimonene nanoribbons and nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 97, 98-104.	1.3	51
9308	Accuracy of dielectric-dependent hybrid functionals in the prediction of optoelectronic properties of metal oxide semiconductors: a comprehensive comparison with many-body GW and experiments. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 044003.	0.7	59
9309	Benchmarking of DFT functionals for the kinetics and mechanisms of atmospheric addition reactions of OH radicals with phenyl and substituted phenyl-based organic pollutants. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25533.	1.0	14
9310	Optical absorption spectra and g factor of MgO: Mn ²⁺ explored by ab initio and semi empirical methods. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 113, 194-200.	1.9	8
9311	Photochemical relaxation pathways of S ⁶ -methylthioinosine and O ⁶ -methylguanosine in solution. <i>Faraday Discussions</i> , 2018, 207, 351-374.	1.6	9
9312	A computational investigation into nickel-bis(diselenolene) complexes as potential catalysts for reduction of H ⁺ to H ₂ . <i>Canadian Journal of Chemistry</i> , 2018, 96, 51-57.	0.6	3
9313	Fluorescent Benzocoumarin-Extended Styryl Hybrids: Solvatochromism, Excess Dipole Moment, NLO Properties and DFT Study. <i>Journal of Fluorescence</i> , 2018, 28, 293-309.	1.3	12

#	ARTICLE	IF	CITATIONS
9314	H ₂ effect in Chevronâ€“Phillips ethylene trimerization catalytic system: an experimental and theoretical investigation. <i>Polymer Bulletin</i> , 2018, 75, 3555-3565.	1.7	8
9315	Effect of mechanical stress on the Raman and infrared bands of hydroxylapatite: A quantum mechanical first principle investigation. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2018, 77, 683-692.	1.5	17
9316	NLOphoric rigid pyrazino-phenanthroline donor-â€“acceptor compounds: Investigation of structural and solvent effects on non-linear optical properties using computational methods. <i>Optical Materials</i> , 2018, 75, 379-389.	1.7	14
9317	Neutral noble gas compound with a xenon-metal double bond: A theoretical study of F ₂ XeWF ₂ . <i>Computational and Theoretical Chemistry</i> , 2018, 1123, 35-40.	1.1	3
9318	Tris(perfluoroalkyl)germylethynyl derivatives of biphenyl containing ferrocenyl donor group: Structure, spectra, and photoinduced intramolecular electron transfer. <i>Computational and Theoretical Chemistry</i> , 2018, 1123, 50-60.	1.1	7
9319	Theoretical molecular design of hexasilabenzene analogues aiming for the thermodynamic and kinetic stabilization. <i>Computational and Theoretical Chemistry</i> , 2018, 1123, 61-72.	1.1	7
9320	Theoretical approach for the performance of 4-mercapto-1-alkylpyridin-1-ium bromide as corrosion inhibitors using DFT. <i>Egyptian Journal of Petroleum</i> , 2018, 27, 695-699.	1.2	31
9321	Infrared spectra of isotopomers of chloromethylene in solid argon. <i>Journal of Molecular Spectroscopy</i> , 2018, 345, 17-21.	0.4	0
9322	Theoretical evaluation of chemical substitutions along the main chain of poly(3-hexylthiethylene-vinylene) for solar cell applications. <i>Polymer International</i> , 2018, 67, 197-203.	1.6	2
9323	Three-Component Synthesis and Photophysical Properties of Novel Coumarin-Based Merocyanines. <i>Chemistry - A European Journal</i> , 2018, 24, 974-983.	1.7	27
9324	Activation of Dinitrogen with a Superalkali Species, Li ₃ F ₂ . <i>ChemPhysChem</i> , 2018, 19, 256-260.	1.0	17
9325	Investigation of NH ₃ adsorption behavior on graphdiyne nanosheet and nanotubes: A first-principles study. <i>Journal of Molecular Liquids</i> , 2018, 249, 24-32.	2.3	65
9326	An improved synthesis, spectroscopic (FT-IR, NMR) study and DFT computational analysis (IR, NMR,) of Molecular Structure, 2018, 1155, 548-560.	1.8	37
9327	The effect of alkyl chain tethers on the kinetics and mechanistic behaviour of bifunctional dinuclear platinum(II) complexes bearing N,N'-dipyridylamine ligands. <i>New Journal of Chemistry</i> , 2018, 42, 214-227.	1.4	7
9328	The mechanism of the reaction between an aziridine and carbon dioxide with no added catalyst. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3735.	0.9	14
9329	Investigation of carboxylation of carbon nanotube in the adsorption of anti-cancer drug: A theoretical approach. <i>Applied Surface Science</i> , 2018, 427, 112-125.	3.1	21
9330	Study of the Vibrational Spectrum of Hydrogen Molecules in an Aerogel. <i>JETP Letters</i> , 2018, 108, 661-663.	0.4	0
9331	Novel equations to predict vibrational spectroscopic and electrodynamic properties of molecules. <i>Journal of Physics Communications</i> , 2018, 2, 045031.	0.5	0

#	ARTICLE	IF	CITATIONS
9332	Anisotropy and directional elastic behavior data obtained from the second-order elastic constants of portlandite Ca(OH) ₂ and brucite Mg(OH) ₂ . Data in Brief, 2018, 21, 1375-1380.	0.5	2
9333	Quantitative Assessment of rPM6 for Fluorine- and Chlorine-Containing Metal Complexes: Comparison with Experimental, First-Principles, and Other Semiempirical Results. Molecules, 2018, 23, 3332.	1.7	1
9334	An Assessment of Computational Methods for Calculating Accurate Structures and Energies of Bio-Relevant Polysulfur/Selenium-Containing Compounds. Molecules, 2018, 23, 3323.	1.7	9
9335	Diversity-Oriented Synthesis and Optical Properties of Bichromophoric Pyrrole-Fluorophore Conjugates. Frontiers in Chemistry, 2018, 6, 579.	1.8	4
9336	Discovery of Novel Topological Materials <i>Via</i> High-throughput Computational Search. , 2018, , 392-422.		1
9337	Tropospheric oxidation of methyl hydrotrioxide (CH ₃ OOH) by hydroxyl radical. Physical Chemistry Chemical Physics, 2018, 20, 27406-27417.	1.3	7
9338	<i>Ab initio</i> molecular dynamics study of solvated electrons in methanol clusters. Physical Chemistry Chemical Physics, 2018, 20, 28741-28750.	1.3	8
9339	Detailed kinetics of tetrafluoroethene ozonolysis. Physical Chemistry Chemical Physics, 2018, 20, 28059-28067.	1.3	4
9340	Asymmetric abstraction of two chemically-equivalent methylene hydrogens: significant enantioselectivity of endoperoxide presented by fumitremorgin B endoperoxidase. Physical Chemistry Chemical Physics, 2018, 20, 26500-26505.	1.3	13
9341	Long-lived triplet excited state in a platinum(ii) perylene monoimide complex. Dalton Transactions, 2018, 47, 15071-15081.	1.6	16
9342	Electron-poor hemilabile dicationic palladium NHC complexes â€“ synthesis, structure and catalytic activity. Dalton Transactions, 2018, 47, 16638-16650.	1.6	12
9343	Reactions of dicobalt octacarbonyl with dinucleating and mononucleating bis(imino)pyridine ligands. Dalton Transactions, 2018, 47, 15353-15363.	1.6	17
9344	3D isomorphous lanthanide coordination polymers displaying magnetic refrigeration, slow magnetic relaxation and tunable proton conduction. Dalton Transactions, 2018, 47, 15405-15415.	1.6	48
9345	Interaction of a gold(ⁱ) dicarbene anticancer drug with human telomeric DNA G-quadruplex: solution and computationally aided X-ray diffraction analysis. Dalton Transactions, 2018, 47, 16132-16138.	1.6	35
9346	Photoinduced energy transfer in carbazoleâ€“BODIPY dyads. Physical Chemistry Chemical Physics, 2018, 20, 27418-27428.	1.3	24
9347	Understanding interactions of organic nitrates with the surface and bulk of organic films: implications for particle growth in the atmosphere. Environmental Sciences: Processes and Impacts, 2018, 20, 1593-1610.	1.7	12
9348	Influence of oddâ€“even effect and intermolecular interactions in 2D molecular layers of bisamide organogelators. RSC Advances, 2018, 8, 35195-35204.	1.7	7
9349	Benzothiadiazoleâ€“ethynylthiophenezoic acid as an acceptor of photosensitizer for efficient organic dye-sensitized solar cells. Journal of Materials Chemistry A, 2018, 6, 21493-21500.	5.2	17

#	ARTICLE	IF	CITATIONS
9350	Molecular Engineering of a New Organic Chromophore with D- π -A Architecture for Dye-Sensitized Solar Cells. <i>Materials Today: Proceedings</i> , 2018, 5, 21498-21504.	0.9	3
9351	Insights into the Base-Assisted Acrylate Formation from CO ₂ /C ₂ H ₄ Coupling by Pd- and Ni-catalyst: A DFT Mechanistic Study. <i>ChemCatChem</i> , 2018, 10, 5669-5678.	1.8	8
9352	Differential Metal Ion Sensing by an Antipyrine Derivative in Aqueous and β -Cyclodextrin Media: Selectivity Tuning by β -Cyclodextrin. <i>Analytical Chemistry</i> , 2018, 90, 13607-13615.	3.2	33
9353	Computational Exploration of a Pd(II)-Catalyzed β -C-H Arylation Where Stereoselectivity Arises from Attractive Aryl-Aryl Interactions. <i>Journal of Organic Chemistry</i> , 2018, 83, 14786-14790.	1.7	8
9354	Heterolytic N-H bond activation of ammonia by dinuclear [M(η^4 -OMe)] ₂ complexes (M = Sc and V and Mn). <i>J. Phys. Chem. B</i> , 2018, 122, 11000-11006.	1.1	6
9355	Electronic structure theory gives insights into the higher efficiency of the PTB electron-donor polymers for organic photovoltaics in comparison with prototypical P3HT. <i>Journal of Chemical Physics</i> , 2018, 149, 184905.	1.2	2
9356	Structural Characteristics, Population Analysis, and Binding Energies of [An(NO ₃) ₂] ²⁺ (with An = Ac to Lr). <i>ACS Omega</i> , 2018, 3, 14127-14143.	1.6	15
9357	Curing basis-set convergence of wave-function theory using density-functional theory: A systematically improvable approach. <i>Journal of Chemical Physics</i> , 2018, 149, 194301.	1.2	33
9358	Local and global interpolations along the adiabatic connection of DFT: a study at different correlation regimes. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 166.	0.5	13
9359	Crystal-chemical and structural data related to the equation of state and second-order elastic constants of portlandite Ca(OH) ₂ and brucite Mg(OH) ₂ . <i>Data in Brief</i> , 2018, 21, 2367-2375.	0.5	3
9360	Assessing Configurational Sampling in the Quantum Mechanics/Molecular Mechanics Calculation of Temoporfin Absorption Spectrum and Triplet Density of States. <i>Molecules</i> , 2018, 23, 2932.	1.7	10
9361	Hybrid Organic-Inorganic Functionalized Dodecaboranes and Their Potential Role in Lithium and Magnesium Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27947-27954.	1.5	7
9362	QTAIM Assessment of the Intra- and Intermolecular Bonding in a Bis(nitramido-oxadiazolate) Energetic Ionic Salt at 20 K. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9676-9687.	1.1	2
9363	Shrinking Self-Interaction Errors with the Fermi- γ Orbital Self-Interaction-Corrected Density Functional Approximation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9307-9315.	1.1	30
9364	Gas-Phase Stereo-inversion in Aspartic Acid: Reaction Pathways, Computational Spectroscopic Analysis, and Its Astrophysical Relevance. <i>ACS Omega</i> , 2018, 3, 14431-14447.	1.6	8
9365	Density functional benchmark studies on structure and energetics of 3d transition metal mononitrides. <i>Journal of Chemical Sciences</i> , 2018, 130, 1.	0.7	6
9366	Incremental embedding: A density matrix embedding scheme for molecules. <i>Journal of Chemical Physics</i> , 2018, 149, 194108.	1.2	17
9367	Synthesis, Characterization and Theoretical Study of the Chemical Reactivity of New Cyclic Sulfamides Linked to Tetrathiafulvalene. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2018, 193, 697-704.	0.8	2

#	ARTICLE	IF	CITATIONS
9368	Reply to: "The diamine cation is not a chemical example where density functional theory fails". Nature Communications, 2018, 9, 5348.	5.8	5
9369	Exploring the Solubility of the Carbamazepine-Saccharin Cocrystal: A Charge Density Study. Crystal Growth and Design, 2021, 21, 4259-4275.	1.4	8
9370	Computational Comparative Mechanistic Study of C ⁺ E (E=C,N,O,S) Coupling Reactions through CO ₂ Activation Mediated by Uranium(III) Complexes. Chemistry - A European Journal, 2018, 24, 19289-19299.	1.7	3
9371	DFT and TD-DFT study of new D-π-A dyes for Grätzel solar cell. AIP Conference Proceedings, 2018, , .	0.3	5
9372	Communication: Strong-interaction limit of an adiabatic connection in Hartree-Fock theory. Journal of Chemical Physics, 2018, 149, 241101.	1.2	25
9373	2-(1,1-dioxidobenzo[b]thiophen-2(2H)-ylidene)malononitrile (BTD) Based Styryl Chromophores: Solvatochromic and Computational Investigation of Linear and NLO properties. ChemistrySelect, 2018, 3, 13654-13664.	0.7	10
9374	First-Principles Study of Point Defects in GaAs/AlAs Superlattice: the Phase Stability and the Effects on the Band Structure and Carrier Mobility. Nanoscale Research Letters, 2018, 13, 301.	3.1	29
9375	A theoretical study of fused thiophene modified anthracene-based organic dyes for dye-sensitized solar cell applications. New Journal of Chemistry, 2018, 42, 20163-20170.	1.4	21
9376	Taking Solution Proton NMR to Its Extreme: Prediction and Detection of a Hydride Resonance in an Intermediate-Spin Iron Complex. Journal of the American Chemical Society, 2018, 140, 17413-17417.	6.6	37
9377	Controlling Nuclearity and Stereochemistry in Vanadyl(V) and Mixed Valent V ^{IV} /V ^V Complexes of Oxido-Pincer Pyridine-2,6-dimethanol Ligands. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2018, 644, 1805-1815.	0.6	3
9378	Influence of Oxygen Vacancy Density on the Polaronic Configuration in Rutile. Materials, 2018, 11, 2156.	1.3	7
9379	Corrosion Inhibition of Carbon Steel by Anthraquinones Derivatives in 1.0 M HCl: Electrochemical and Quantum Calculations. International Journal of Electrochemical Science, 2018, , 5096-5119.	0.5	7
9380	Structures of the neutral and positively charged forms of the 4,4'-bis(4'-tris(N,N-phenyl-3-methylphenylamino)triphenylamine (m-MTDATA) molecule and its dimer, and charge localization in the corresponding cationic species. Journal of Molecular Modeling, 2018, 24, 345.	0.8	1
9381	Structural, Optical, and Magnetic Properties of Ultramarine Pigments: A DFT Insight. Journal of Physical Chemistry C, 2018, 122, 29338-29349.	1.5	8
9382	Performance of Density-Functional Tight-Binding in Comparison to Ab Initio and First-Principles Methods for Isomer Geometries and Energies of Glucose Epimers in Vacuo and Solution. ACS Omega, 2018, 3, 16899-16915.	1.6	12
9383	Post-transition state bifurcations induce dynamical detours in Pummerer-like reactions. Chemical Science, 2018, 9, 8937-8945.	3.7	45
9384	Effective corrosion inhibition of mild steel in acidic medium using inexpensive kermes natural dye: experimental and quantum chemical study. Anti-Corrosion Methods and Materials, 2018, 65, 626-636.	0.6	8
9385	Competitive McLafferty-type rearrangements of sodium adduct of anti-2,3-dihydroxy-1-phenylpentane-1,4-dione compounds in tandem mass spectrometry. European Journal of Mass Spectrometry, 2018, 24, 437-441.	0.5	3

#	ARTICLE	IF	CITATIONS
9386	Anionic Germanium ^{II} -Niobium Clusters: Atomic Structure, Mechanisms of Cluster Formation, and Electronic Spectra. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 1720-1726.	0.1	7
9387	Structure and dynamics of <i>Helicobacter pylori</i> nickel-chaperone HypA: an integrated approach using NMR spectroscopy, functional assays and computational tools. <i>Journal of Biological Inorganic Chemistry</i> , 2018, 23, 1309-1330.	1.1	20
9388	Achieving High Efficiency in Solution-Processed Perovskite Solar Cells Using C ₆₀ /C ₇₀ Mixed Fullerenes. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 39590-39598.	4.0	67
9389	Unraveling the spectral signatures of solvent ordering in K-edge XANES of aqueous Na ⁺ . <i>Journal of Chemical Physics</i> , 2018, 149, 124503.	1.2	12
9390	Mechanistic studies: enantioselective palladium(^{II})-catalyzed intramolecular aminoarylation of alkenes by dual N-H and aryl C-H bond cleavage. <i>Organic Chemistry Frontiers</i> , 2018, 5, 3256-3262.	2.3	4
9391	Absorption Characteristics of Combination Medication of Realgar and Indigo Naturalis: In Vitro Transport across MDCK-MDR1 Cells and In Vivo Pharmacokinetics in Mice after Oral Administration. <i>Evidence-based Complementary and Alternative Medicine</i> , 2018, 2018, 1-10.	0.5	4
9392	Analysis of degradation products of nerve agents via post-pentafluorobenzoylation liquid chromatography-tandem mass spectrometry. <i>Journal of Chromatography A</i> , 2018, 1577, 31-37.	1.8	14
9393	Quantum-Chemical Insights into the Phosphorescence Efficiencies of Blue-Emitting Platinum Complexes with Phenylene-Bridged Pincer Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 12174-12186.	1.9	11
9394	Computational design of a molecular triple photoswitch for wavelength-selective control. <i>Chemical Science</i> , 2018, 9, 8665-8672.	3.7	29
9395	Synthesis, Crystal Structures and Magnetic Properties of Two Heterobridged μ -Phenoxo μ -1,1-Azide/Isocyanate Dinickel(II) Compounds: Experimental and Theoretical Exploration. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 4556-4565.	1.0	11
9396	Cascade radical cyclization/cross-coupling of halobenzamides by synergistic Cu/Fe catalysis: An access to 7-tert-alkylated isoquinolinediones. <i>Tetrahedron</i> , 2018, 74, 6558-6568.	1.0	10
9397	Theoretical Investigations on the Structural, Electronic and Spectral Properties of VF _n (n = 1-7) Clusters. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2018, 73, 1091-1104.	0.7	7
9398	Reactivity Indexes and Structure of Fullerenes. , 2018, , .		0
9399	Corrosion Resistance of Mild Steel Coated with Organic Material Containing Pyrazol Moiety. <i>Coatings</i> , 2018, 8, 330.	1.2	42
9400	Mechanisms of Antioxidant Activities of Fullerenols from First-Principles Calculation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8183-8190.	1.1	27
9401	Theoretical study of triphenylamine-based organic dyes with mono-, di-, and tri-anchoring groups for dye-sensitized solar cells. <i>Organic Electronics</i> , 2018, 63, 328-342.	1.4	48
9402	Effect of Structure on the Spin-Spin Interactions of Tethered Dicyanomethyl Diradicals. <i>Journal of the American Chemical Society</i> , 2018, 140, 14308-14313.	6.6	31
9403	Tungsten-Embedded Graphene: Theoretical Study on a Potential High-Activity Catalyst toward CO Oxidation. <i>Materials</i> , 2018, 11, 1848.	1.3	13

#	ARTICLE	IF	CITATIONS
9404	Spectral Calculations with DFT. , 0, , .		5
9405	Conformational Features of Thioamide-Containing Dipeptoids and Peptoidâ€“Peptide Hybridsâ€“Computational and Experimental Approaches. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7819-7831.	1.1	2
9406	Structure-Based Theory of Fluctuation-Induced Energy Transfer in a Molecular Dyad. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5940-5947.	2.1	15
9407	Luminescent Zn(ii) coordination polymers as efficient fluorescent sensors for highly sensitive detection of explosive nitroaromatics. <i>CrystEngComm</i> , 2018, 20, 6762-6774.	1.3	32
9408	Theoretical Studies on Catalysis Mechanisms of Serum Paraoxonase 1 and Phosphotriesterase Diisopropyl Fluorophosphatase Suggest the Alteration of Substrate Preference from Paraoxonase to DFP. <i>Molecules</i> , 2018, 23, 1660.	1.7	7
9409	A combined experimental/theoretical approach to accelerated fuel cell development by quantitative prediction of redox potentials. <i>Journal of Power Sources</i> , 2018, 399, 443-447.	4.0	2
9410	Oxidation of amino acids by peracetic acid: Reaction kinetics, pathways and theoretical calculations. <i>Water Research X</i> , 2018, 1, 100002.	2.8	75
9411	Stability and Electronic Properties of Rocksalt (CdO) _n , (SrO) _n , and (BaO) _n Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2018, 122, 25021-25034.	1.5	6
9412	Quantum Chemical Study of Niobium and Tantalum M4O10 Oxide Clusters and M4O 10 â€“ Anions. <i>Russian Journal of General Chemistry</i> , 2018, 88, 622-625.	0.3	2
9413	A structural DFT study of MM, GG, MG, and GM alginic acid disaccharides and reactivity of the MG metallic complexes. <i>Journal of Molecular Modeling</i> , 2018, 24, 312.	0.8	16
9414	Ligand-Assisted Metal-Centered Electrocatalytic Hydrogen Evolution upon Reduction of a Bis(thiosemicarbazonato)Ni(II) Complex. <i>Inorganic Chemistry</i> , 2018, 57, 13486-13493.	1.9	58
9415	Lessons from the Spin-Polarization/Spin-Contamination Dilemma of Transition-Metal Hyperfine Couplings for the Construction of Exchange-Correlation Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5653-5672.	2.3	35
9416	The Shape of Native Plant Cellulose Microfibrils. <i>Scientific Reports</i> , 2018, 8, 13983.	1.6	86
9417	Protonation and Reduction of the FeMo Cluster in Nitrogenase Studied by Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6653-6678.	2.3	52
9418	Davydov-type excitonic effects on the absorption spectra of parallel-stacked and herringbone aggregates of pentacene: Time-dependent density-functional theory and time-dependent density-functional tight binding. <i>Journal of Chemical Physics</i> , 2018, 149, 134111.	1.2	17
9419	Spectroscopy and DFT Calculations of Flavoâ€“Diiron Nitric Oxide Reductase Identify Bridging Structures of NO-Coordinated Diiron Intermediates. <i>ACS Catalysis</i> , 2018, 8, 11704-11715.	5.5	20
9420	Polymorphism, Crystal Packing, Twinning, and Molecular Conformations in 5â€“Halo-5â€“deoxyguanosines and a Hydrate of the Pseudohalide Analogue, 5â€“Azido-5â€“deoxyguanosine. <i>Crystal Growth and Design</i> , 2018, 18, 6995-7005.	1.4	0
9421	Modeling Ammonia and Water Co-Adsorption in CuI-SSZ-13 Zeolite Using DFT Calculations. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 15982-15990.	1.8	7

#	ARTICLE	IF	CITATIONS
9422	Theoretical simulation of the Qx-band absorption and fluorescence spectra of cis-isobacteriochlorin: Including the Duschinsky and Herzberg-Teller effects. <i>Chemical Physics Letters</i> , 2018, 713, 215-225.	1.2	2
9423	Theoretical Study of Alkylsulfonic Acids: Force-Field Development and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9747-9756.	1.2	1
9426	Structures and magnetic properties of small Co_n^+ and Co_n^{2+} ($n=1-5$) clusters. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 474002.		
9427	Chemical shift reference scale for Li solid state NMR derived by first-principles DFT calculations. <i>Journal of Magnetic Resonance</i> , 2018, 297, 33-41.	1.2	14
9428	Accuracy of theoretical catalysis from a model of iron-catalyzed ammonia synthesis. <i>Communications Chemistry</i> , 2018, 1, .	2.0	11
9429	(+)-Dimeric biscognienyne A: Total Synthesis and Mechanistic Investigations of the Key Heterodimerization. <i>Organic Letters</i> , 2018, 20, 6886-6890.	2.4	21
9430	Mechanism of the Visible-Light-Mediated Copper-Catalyzed Coupling Reaction of Phenols and Alkynes. <i>Journal of the American Chemical Society</i> , 2018, 140, 15099-15113.	6.6	50
9431	Base-free benzylation of 1,3-dicarbonyl compounds using sulfamic acid supported on silica by linker: a combined experimental and theoretical approach. <i>Monatshefte für Chemie</i> , 2018, 149, 2237-2244.	0.9	4
9432	Range-Separated Hybrid Functionals with Variational Fitted Exact Exchange. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5608-5616.	2.3	17
9433	Stereoselectivity, Different Oxidation States, and Multiple Spin States in the Cyclopropanation of Olefins Catalyzed by Fe-Porphyrin Complexes. <i>ACS Catalysis</i> , 2018, 8, 11140-11153.	5.5	27
9434	A theoretical study on the coordination behavior of some phosphoryl, carbonyl and sulfoxide derivatives in lanthanide complexation. <i>Journal of Molecular Modeling</i> , 2018, 24, 328.	0.8	5
9435	On the performance of DFT/MRCI Hamiltonians for electronic excitations in transition metal complexes: The role of the damping function. <i>Journal of Chemical Physics</i> , 2018, 149, 164106.	1.2	42
9436	Samarium cation (Sm^+) reactions with H_2 , D_2 , and HD : SmH^+ bond energy and mechanistic insights from guided ion beam and theoretical studies. <i>Journal of Chemical Physics</i> , 2018, 149, 164304.	1.2	7
9437	An automated framework for NMR chemical shift calculations of small organic molecules. <i>Journal of Cheminformatics</i> , 2018, 10, 52.	2.8	37
9438	The Structural Signs of Sweetness in Artificial Sweeteners: A Rotational Study of Sorbitol and Dulcitol. <i>ChemPhysChem</i> , 2018, 19, 3334-3340.	1.0	16
9439	Enantioselective Vanadium-Catalyzed Oxidative Coupling: Development and Mechanistic Insights. <i>Journal of Organic Chemistry</i> , 2018, 83, 14362-14384.	1.7	42
9440	Assessment of a range-separated orbital-optimised random-phase approximation electron correlation method. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	6
9441	Aggregation-Induced Emission in Phenothiazine-TPE and TPAN Polymers. <i>Macromolecules</i> , 2018, 51, 8501-8512.	2.2	39

#	ARTICLE	IF	CITATIONS
9442	A Stable Trimethylenemethane Triplet Diradical Based on a Trimeric Porphyrin Fused π - σ System. <i>Angewandte Chemie</i> , 2018, 130, 9635-9638.	1.6	17
9443	A Density Functional Theory Study on the Diffusion of Fission Gas Atoms in Uranium Dioxide. <i>Journal of Nuclear Engineering and Radiation Science</i> , 2018, 4, .	0.2	1
9444	Decomposition of d- and f-Shell Contributions to Uranium Bonding from the Quantum Theory of Atoms in Molecules: Application to Uranium and Uranyl Halides. <i>Inorganics</i> , 2018, 6, 88.	1.2	19
9445	The tardy dance of molecular orbitals. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25718.	1.0	3
9446	Ligation state of nickel during C O bond activation with monodentate phosphines. <i>Tetrahedron</i> , 2018, 74, 6717-6725.	1.0	17
9447	Isothermal Titration Calorimetry for the Screening of Aflatoxin B1 Surface-Enhanced Raman Scattering Sensor Affinity Agents. <i>Analytical Chemistry</i> , 2018, 90, 13409-13418.	3.2	18
9448	Experimental and theoretical insights into the electrooxidation pathway of azo-colorants on glassy carbon electrode. <i>Electrochimica Acta</i> , 2018, 290, 556-567.	2.6	23
9449	Energy Decomposition Analysis for Excimers Using Absolutely Localized Molecular Orbitals within Time-Dependent Density Functional Theory and Configuration Interaction with Single Excitations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5156-5168.	2.3	22
9450	Mechanism and Kinetics of the Gas-Phase Stereoconversion in Proteinogenic L-Threonine and Its Astrophysical Relevance. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7572-7586.	1.1	8
9451	Controlling Isomerization Selectivity in Chiral, Photochromic N,C-Chelate Organoboron Systems with Extended π -Conjugation. <i>Journal of Organic Chemistry</i> , 2018, 83, 11970-11977.	1.7	12
9452	Using Theory To Reinterpret the Kinetics of Monofunctional Platinum Anticancer Drugs: Stacking Matters. <i>Journal of the American Chemical Society</i> , 2018, 140, 14024-14027.	6.6	35
9453	Computational study on palladium-catalyzed alkenylation of remote $\hat{C}(sp^3)C-H$ bonds with alkynes: a new understanding of mechanistic insight and origins of site-selectivity. <i>RSC Advances</i> , 2018, 8, 30186-30190.	1.7	4
9454	Effects of Mechanical Stretching on the Properties of Conjugated Polymers: Case Study for MEH-PPV and P3HT Oligomers. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2018, 56, 1413-1426.	2.4	11
9455	Synthesis of Nonaromatic and Aromatic Dithia Benzisapphyrins. <i>Journal of Organic Chemistry</i> , 2018, 83, 11794-11803.	1.7	28
9456	Electron transfer characteristics of 2-deoxy-2-fluoro-arabinonucleic acid, a nucleic acid with enhanced chemical stability. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26063-26067.	1.3	8
9457	Quantum chemistry study on regioselectivity in ruthenium catalyzed synthesis of 1,5-disubstituted 1,2,3-triazoles. <i>Computational and Theoretical Chemistry</i> , 2018, 1143, 29-35.	1.1	7
9458	QM and ONIOM studies on thermally activated delayed fluorescence of copper(σ) complexes in gas phase, solution, and crystal. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 24955-24967.	1.3	30
9459	Avian Magnetoreception. <i>Springer Theses</i> , 2018, , 83-107.	0.0	0

#	ARTICLE	IF	CITATIONS
9460	Computational, experimental details, and biological raw data accompanying the publication: "The synthesis and characterization of a nanomagnetite with potent antibacterial activity and low mammalian toxicity". Data in Brief, 2018, 21, 2518-2521.	0.5	8
9461	Theoretical investigation of gold(I)-catalyzed intramolecular SEAr in isoxazole derivatives: Mechanisms, origin of regioselectivity, and role of hydrogen acceptor. Molecular Catalysis, 2018, 460, 27-35.	1.0	11
9462	Reaction Mechanism and Thermodynamic Properties of Aliphatic Hydrocarbon Groups during Coal Self-Heating. Energy & Fuels, 2018, 32, 10469-10477.	2.5	36
9463	Unraveling substituent effects on frontier orbitals of conjugated molecules using an absolutely localized molecular orbital based analysis. Chemical Science, 2018, 9, 8598-8607.	3.7	46
9464	Theoretical Study on Structures and Stabilities of N ₇ C _R (<i>R</i> =H,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 582 Td	0.7	1
9465	Synthesis of <i>meso</i> -Tetraaryl Triphyrins(2.1.1). Journal of Organic Chemistry, 2018, 83, 12945-12950.	1.7	28
9466	Microscopic Origin of Different Hydration Patterns of <i>para</i> -Nitrophenol and Its Anion: A Study Combining Multiconfigurational Calculations and the Free-Energy Gradient Method. Journal of Physical Chemistry B, 2018, 122, 9202-9209.	1.2	4
9467	Target-based drug discovery through inversion of quantitative structure-drug-property relationships and molecular simulation: CA IX-sulphonamide complexes. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 1430-1443.	2.5	14
9468	Exploring Oxidation State-Dependent Selectivity in Polymerization of Cyclic Esters and Carbonates with Zinc(II) Complexes. IScience, 2018, 7, 120-131.	1.9	13
9469	Accessing Two-Stage Regioselective Photoisomerization in Unsymmetrical N,C-Chelate Organoboron Compounds: Reactivity of B(ppz)(Mes)Ar. Organometallics, 2018, 37, 3360-3367.	1.1	9
9470	Revised M06 density functional for main-group and transition-metal chemistry. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10257-10262.	3.3	144
9471	Photoelectron spectra of copper oxide cluster anions from first principles methods. Journal of Chemical Physics, 2018, 149, 064306.	1.2	8
9472	Pseudo-tetrahedral Rhodium and Iridium Complexes: Catalytic Synthesis of <i>E</i> -Enynes. Chemistry - A European Journal, 2018, 24, 17545-17556.	1.7	7
9473	Computational exploration of Pd-catalyzed C-H bond activation reactions. International Journal of Quantum Chemistry, 2018, 118, e25723.	1.0	11
9474	Theoretical investigation of the sensing mechanism of the pure graphene and AL,B,N,P doped mono-vacancy graphene-based methane. Chemical Physics Letters, 2018, 710, 221-225.	1.2	19
9475	Do Semilocal Density-Functional Approximations Recover Dispersion Energies at Small Intermonomer Separations?. Physical Review Letters, 2018, 121, 113402.	2.9	33
9476	Covalently Linked <i>meso</i> -BODIPYnyl Dithiahomoporphyrins: Synthesis and Properties. European Journal of Organic Chemistry, 2018, 2018, 5389-5396.	1.2	11
9477	Theoretical design of metal-phthalocyanine dye-sensitized solar cells with improved efficiency. Journal of Molecular Modeling, 2018, 24, 279.	0.8	8

#	ARTICLE	IF	CITATIONS
9496	A new class of triphenylamine-based novel sensitizers for DSSCs: a comparative study of three different anchoring groups. <i>New Journal of Chemistry</i> , 2018, 42, 11555-11564.	1.4	37
9497	Surface chemistry of thermal dry etching of cobalt thin films using hexafluoroacetylacetone (hfach). <i>Applied Surface Science</i> , 2018, 455, 438-445.	3.1	21
9498	Effects of substitutions in the equatorial position on the stabilities of pentacoordinated silicon anions of $\text{ClSi}(\text{abc})\text{OCl}$ ($\text{a}, \text{b}, \text{c} = \text{H}, \text{F}, \text{Cl}$) from theoretical investigation. <i>Journal of the Chinese Chemical Society</i> , 2018, 65, 1179-1187.	0.8	1
9499	Mapping Bridge Conformational Effects on Electronic Coupling in Mo_2 Mixed-Valence Systems. <i>Inorganic Chemistry</i> , 2018, 57, 7455-7467.	1.9	13
9500	Performance of various density-functional approximations for cohesive properties of 64 bulk solids. <i>New Journal of Physics</i> , 2018, 20, 063020.	1.2	185
9501	Highly efficient carbazole based co-sensitizers carrying electron deficient barbituric acid for NCSU-10 sensitized DSSCs. <i>Solar Energy</i> , 2018, 169, 386-391.	2.9	27
9502	Neural network for prediction of ^{13}C NMR chemical shifts of fullerene C_{60} monoadducts. <i>Journal of Chemometrics</i> , 2018, 32, e3037.	0.7	2
9503	Mechanistic Insights into the Ni-Catalyzed Reductive Carboxylation of $\text{C}=\text{O}$ Bonds in Aromatic Esters with CO_2 : Understanding Remarkable Ligand and Traceless-Directing-Group Effects. <i>Chemistry - an Asian Journal</i> , 2018, 13, 1570-1581.	1.7	5
9504	Possibility of reducing the coordinated dinitrogen into ammonia and hydrazine using $[\text{Ru-L}]$ ($\text{L} = \text{Tj ETQqO O O rgBT/Overlock 10 Tf 50 4}$)	0.7	10
9505	Microwave-Assisted Method for the Synthesis of Perylene Ester Imides as a Gateway Toward Unsymmetrical Perylene Bisimides. <i>Journal of Organic Chemistry</i> , 2018, 83, 6290-6300.	1.7	16
9506	Near-Infrared Fluorescence from In-Plane-Aromatic Cycloparaphenylene Dications. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5162-5167.	1.1	20
9507	Exploring the Limitation of Molecular Water Oxidation Catalysts. <i>Journal of Physical Chemistry C</i> , 2018, 122, 12404-12412.	1.5	37
9508	How does binuclear zinc amidohydrolase FwdA work in the initial step of methanogenesis: From formate to formyl-methanofuran. <i>Journal of Inorganic Biochemistry</i> , 2018, 185, 71-79.	1.5	2
9509	Highly Stoke shifted near infrared (NIR) emitting donor-pi-acceptor chromophore: Synthesis and combined experimental and computational studies of photophysical properties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 363, 13-22.	2.0	8
9510	Restoring Size Consistency of Approximate Functionals Constructed from the Adiabatic Connection. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3137-3142.	2.1	26
9511	Theoretical insight in highly luminescent properties of Eu(III) complex with phenanthroline. <i>Journal of Luminescence</i> , 2018, 202, 192-205.	1.5	28
9512	Koopmans-Compliant Spectral Functionals for Extended Systems. <i>Physical Review X</i> , 2018, 8, .	2.8	34
9513	Insights into geometries, stabilities, electronic structures, reactivity descriptors, and magnetic properties of bimetallic Ni_mCu_n ($m = 1, 2; n = 3-13$) clusters: Comparison with pure copper clusters. <i>Journal of Computational Chemistry</i> , 2018, 39, 1878-1889.		10

#	ARTICLE	IF	CITATIONS
9514	A Thermodynamic Model for ZrO ₂ (am) Solubility at 25 °C in the Ca ²⁺ -Na ⁺ -H ⁺ -Cl ⁻ -OH ⁻ -H ₂ O System: A Critical Review. <i>Journal of Solution Chemistry</i> , 2018, 47, 855-891.	0.6	11
9515	Revisiting electronic nature and geometric parameters of cyclophanes and their relation with stability – DFT, QTAIM and NCI study. <i>Computational and Theoretical Chemistry</i> , 2018, 1135, 18-27.	1.1	4
9516	Effects of meta or para connected organic dyes for dye-sensitized solar cell. <i>Dyes and Pigments</i> , 2018, 158, 165-174.	2.0	40
9517	Polyoxoniobates as a superior Lewis base efficiently catalyzed Knoevenagel condensation. <i>Molecular Catalysis</i> , 2018, 453, 93-99.	1.0	55
9518	Redox-triggered chiroptical switching activity of ruthenium(III)-bis(1,2-diketonato) complexes bearing a bipyridine-chelicene ligand. <i>Chirality</i> , 2018, 30, 592-601.	1.3	12
9519	Design of novel phenanthrocarbazole dyes for efficient applications in dye-sensitized solar cells. <i>Computational Materials Science</i> , 2018, 151, 34-40.	1.4	15
9520	Chemical Bond Energies of 3d Transition Metals Studied by Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3479-3492.	2.3	64
9521	Combined spectroscopic and TDDFT study of single-double anthocyanins for application in dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2018, 42, 11616-11628.	1.4	17
9522	A Comprehensive Assessment of the Effectiveness of Orbital Optimization in Double-Hybrid Density Functionals in the Treatment of Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5610-5624.	1.1	19
9523	Electronic structure and nonlinear optical properties of organic photovoltaic systems with potential applications on solar cell devices: a DFT approach. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	17
9524	Benchmark of different charges for prediction of the partitioning coefficient through the hydrophilic/lipophilic index. <i>Journal of Molecular Modeling</i> , 2018, 24, 141.	0.8	18
9525	Double Molecular Photoswitch Driven by Light and Collisions. <i>Physical Review Letters</i> , 2018, 120, 223002.	2.9	24
9526	Influence of electron donors in fluorescent NLOphoric D- π -A derivatives with acenaphthene rotor: Photophysical, viscosity, and TD-DFT studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 364, 40-52.	2.0	5
9527	Some structural aspects of ammeline – Keto preference and dimerization. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 202, 87-92.	2.0	3
9528	The role of sulfate in the chemical synthesis of graphene oxide. <i>Materials Chemistry and Physics</i> , 2018, 215, 203-210.	2.0	12
9529	Structural Characterization and Photochemical Properties of Mono- and Bimetallic Cu-Mabiq Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 6401-6409.	1.9	6
9530	Density Functional Theory for Microwave Spectroscopy of Noncovalent Complexes: A Benchmark Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4894-4901.	1.1	20
9531	QM/MM studies on ozonolysis of β -humulene and Criegee reactions with acids and water at air-water/acetonitrile interfaces. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16138-16150.	1.3	9

#	ARTICLE	IF	CITATIONS
9532	Solvent-induced ion separation of a beryllium scorpionate complex. <i>Dalton Transactions</i> , 2018, 47, 12511-12515.	1.6	8
9533	Relative stability between the manganese hydroxide- and oxo-models for water oxidation by CCSD, DMRG CASCI, CASSCF, CASPT2 and CASDFT methods; Importance of static and dynamical electron correlation effects for OEC of PSII. <i>Chemical Physics Letters</i> , 2018, 705, 85-91.	1.2	10
9534	New cyanopyridine based conjugative polymers as blue emitters: Synthesis, photophysical, theoretical and electroluminescence studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 364, 6-15.	2.0	11
9535	Photophysical Properties of Novel Two-Photon Absorbing Dyes: Assessing Their Possible Use for Singlet Oxygen Generation. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16315-16324.	1.5	14
9536	An improved model to calculate equilibrium constants for formation of peroxy radical-water complexes. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	3
9537	Design, synthesis, molecular modeling, and biological evaluation of novel β -aminophosphonates based quinazolinone moiety as potential anticancer agents: DFT, NBO and vibrational studies. <i>Journal of Molecular Structure</i> , 2018, 1173, 128-141.	1.8	28
9538	Spectroscopic and DFT assessment of bridging ligand effect on the structural and electronic properties of dinuclear iridium- and rhodium-based complexes. <i>Inorganica Chimica Acta</i> , 2018, 482, 299-306.	1.2	5
9539	Theoretical investigation of Banert cascade reaction. <i>Royal Society Open Science</i> , 2018, 5, 171075.	1.1	7
9540	Elucidating the mass spectrum of the retronecine alkaloid using DFT calculations. <i>Journal of Mass Spectrometry</i> , 2018, 53, 934-941.	0.7	5
9541	Optical nonlinearity and charge transfer analysis of 4-[(E)-2-(2,4,6-Trinitrophenyl) ethylidene] benzonitrile adsorbed on silver nanoparticles: Computational and experimental investigations. <i>Optics and Laser Technology</i> , 2018, 107, 454-467.	2.2	7
9542	Isomerization of hydrocarbons over Pt supported on micro-mesoporous ZSM-5. <i>Polyhedron</i> , 2018, 154, 314-324.	1.0	20
9543	Reaction of CO ₂ with Atomic Transition Metal M ⁺ⁿ Ions: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5848-5860.	1.1	10
9544	A computational mechanistic study of substrate-controlled competitive O-H and C-H insertion reactions catalyzed by dirhodium(<i>sc</i>) carbenoids: insight into the origin of chemoselectivity. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2353-2363.	2.3	9
9545	Gas-phase intramolecular hydroxyl-amino exchange of protonated arginine and verified by the synthetic intermediate compound. <i>Journal of Mass Spectrometry</i> , 2018, 53, 700-704.	0.7	5
9546	Computational modeling of heterogeneous Ziegler-Natta catalysts for olefins polymerization. <i>Progress in Polymer Science</i> , 2018, 84, 89-114.	11.8	120
9547	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17705-17713.	1.3	21
9548	Theory of electron, phonon and spin transport in nanoscale quantum devices. <i>Nanotechnology</i> , 2018, 29, 373001.	1.3	60
9549	Coordination numbers in hydrated Cu(II) ions. <i>Journal of Molecular Modeling</i> , 2018, 24, 187.	0.8	10

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9550	Water catalyzed pyrolysis of oxygen functional groups of coal: A density functional theory investigation. <i>Fuel</i> , 2018, 233, 328-335.	3.4	13
9551	A Series of 4- and 5-Coordinate Ni(II) Complexes: Synthesis, Characterization, Spectroscopic, and DFT Studies. <i>Inorganic Chemistry</i> , 2018, 57, 8307-8316.	1.9	24
9552	Structural evolution and bonding properties of Au ₂ Si ⁿ⁺ /O (n = 1-7) clusters: Anion photoelectron spectroscopy and theoretical calculations. <i>Journal of Chemical Physics</i> , 2018, 148, 244306.	1.2	33
9553	Transition State Search Using rPM6: Iron- and Manganese-Catalyzed Oxidation Reactions as a Test Case. <i>Bulletin of the Chemical Society of Japan</i> , 2018, 91, 1377-1389.	2.0	4
9554	A reference data set for validating vapor pressure measurement techniques: homologous series of polyethylene glycols. <i>Atmospheric Measurement Techniques</i> , 2018, 11, 49-63.	1.2	41
9555	Hydrogen Bonding Regulates the Rigidity of Liposome-Encapsulated Chlorin Photosensitizers. <i>ChemistryOpen</i> , 2018, 7, 475-483.	0.9	13
9556	Solvation of Al ³⁺ cations in bulk and confined protic ionic liquids: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19071-19081.	1.3	15
9557	Kinetic study, structural analysis and computational investigation of novel xerogel based on drug-PEG/SiO ₂ for controlled release of enrofloxacin. <i>Journal of Molecular Liquids</i> , 2018, 266, 733-742.	2.3	14
9558	Exploiting Coordinate Scaling Relations To Accelerate Exact Exchange Calculations. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3886-3890.	2.1	8
9559	A Stable Trimethylenemethane Triplet Diradical Based on a Trimeric Porphyrin Fused System. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 9491-9494.	7.2	42
9560	A quantum theory investigation on atmospheric oxidation mechanisms of acrylic acid by OH radical and its implication for atmospheric chemistry. <i>Environmental Science and Pollution Research</i> , 2018, 25, 24939-24950.	2.7	9
9561	Highly fluorescent blue-green emitting phenanthroimidazole derivatives: Detail experimental and DFT study of structural and donating group effects on fluorescence properties. <i>Dyes and Pigments</i> , 2018, 159, 209-221.	2.0	20
9562	Reactivity of Rhodium(II) amido/Rhodium(I) aminyl complexes. <i>Inorganica Chimica Acta</i> , 2018, 482, 709-716.	1.2	1
9563	Total Stereoselective Michael Addition of N- and S- Nucleophiles to a d-Erythrosyl 1,5-Lactone Derivative. <i>Experimental and Theoretical Studies Devoted to the Synthesis of 2,6-Dideoxy-4-functionalized-d-ribo-1,4-lactone</i> . <i>Journal of Organic Chemistry</i> , 2018, 83, 8011-8019.	1.7	3
9564	Tuning the Photophysical and Electroluminescence Properties in Asymmetrically Tetrasubstituted Bipolar Carbazoles by Functional Group Disposition. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 24013-24027.	4.0	45
9565	Molecular vibration as a novel explanatory mechanism for the expression of animal colouration. <i>Integrative Biology (United Kingdom)</i> , 2018, 10, 464-473.	0.6	5
9566	Band structures in coupled-cluster singles-and-doubles Green's function (GFCCSD). <i>Journal of Chemical Physics</i> , 2018, 148, 204109.	1.2	20
9567	Experimental (FT-IR, Laser-Raman and NMR) and theoretical comparative study on 2-benzylsulfanyl-4-pentyl-6-(phenylsulfanyl)pyrimidine-5-carbonitrile, a potential bioactive agent. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1850035.	1.8	3

#	ARTICLE	IF	CITATIONS
9568	Polymerization of ϵ -Caprolactone Using Bis(phenoxy)-amine Aluminum Complex: Deactivation by Lactide. <i>Inorganic Chemistry</i> , 2018, 57, 10170-10179.	1.9	9
9569	Detection and follow-up reactions of distonic $\langle i \rangle \hat{1}^2 \langle /i \rangle, \langle i \rangle \hat{2}^2 \langle /i \rangle$ -dimesityl enol radical cations containing nitrogen heterocyclic bases. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3865.	0.9	1
9570	Quantum Chemical Calculations and Statistical Analysis: Structural Cytotoxicity Relationships of some Synthesized 2-thiophen-naphtho(benzo)oxazinone Derivatives. <i>Cell Biochemistry and Biophysics</i> , 2018, 76, 377-389.	0.9	1
9571	Activation mechanism of hydrogen peroxide by a divanadium-substituted polyoxometalate $[\text{PV}_2\text{W}_{10}\text{O}_{38}(\frac{1}{4}\text{OH})_2]^{3-}$: A computational study. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 138, 56-67.	1.3	3
9572	Gas-Phase Electron-Impact Activation of Atomic Layer Deposition (ALD) Precursors: MeCpPtMe_3 . <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4602-4606.	2.1	11
9573	Surface terminations of hematite ($\langle i \rangle \hat{1} \langle /i \rangle\text{-Fe}_2\text{O}_3$) exposed to oxygen, hydrogen, or water: dependence on the density functional theory methodology. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 275002.	0.7	16
9574	[4]Cyclofluorene: Unexpected Influence of Alkyl Chain Length. <i>ChemPlusChem</i> , 2018, 83, 874-880.	1.3	28
9575	Wavefunction-like Correlation Model for Use in Hybrid Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4590-4599.	2.3	3
9576	In-situ formation of catalytically active graphene in ethylene photo-epoxidation. <i>Nature Communications</i> , 2018, 9, 3056.	5.8	37
9577	Thermal azide-alkene cycloaddition reactions: straightforward multi-gram access to $\hat{1}^{2,3}$ -1,2,3-triazolines in deep eutectic solvents. <i>Green Chemistry</i> , 2018, 20, 4023-4035.	4.6	30
9578	DFT/TD-DFT study on halogen doping and solvent contributions to the structural and optoelectronic properties of poly[3,6-carbazole] and poly[indolo(3,2-b)-carbazole]. <i>Structural Chemistry</i> , 2018, 29, 1775-1796.	1.0	8
9579	Stereodivergent Rhodium(III)-Catalyzed cis-Cyclopropanation Enabled by Multivariate Optimization. <i>Journal of the American Chemical Society</i> , 2018, 140, 9587-9593.	6.6	55
9580	London dispersion as important factor for the stabilization of $\langle i \rangle Z \langle /i \rangle$ -azobenzenes in the presence of hydrogen bonding. <i>Beilstein Journal of Organic Chemistry</i> , 2018, 14, 1238-1243.	1.3	14
9581	Amido Complexes of Iridium with a PNP Pincer Ligand: Reactivity toward Alkynes and Hydroamination Catalysis. <i>Organometallics</i> , 2018, 37, 2618-2629.	1.1	13
9582	Evaluation of Gas-to-Liquid 17O Chemical Shift of Water: A Test Case for Molecular and Periodic Approaches. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4041-4051.	2.3	2
9583	Quasiparticle energy spectra of isolated atoms from coupled-cluster singles and doubles (CCSD): Comparison with exact CI calculations. <i>Journal of Chemical Physics</i> , 2018, 149, 034106.	1.2	11
9584	Atmospheric fate of methyl pivalate: OH/Cl-initiated degradation and the roles of water and formic acid. <i>Environmental Chemistry</i> , 2018, 15, 246.	0.7	0
9585	Local vertex corrections from exchange-correlation kernels with a discontinuity. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	5

#	ARTICLE	IF	CITATIONS
9586	3- <i>n</i> -Cyano Imidazopyridine Acceptor-based Bipolar and <i>n</i> -type Host Materials for Phosphorescent Organic Light-Emitting Diodes. <i>Asian Journal of Organic Chemistry</i> , 2018, 7, 2218-2222.	1.3	5
9587	Nitrogen Containing Linear Poly(phenylene) Derivatives for Photo-catalytic Hydrogen Evolution from Water. <i>Chemistry of Materials</i> , 2018, 30, 5733-5742.	3.2	88
9588	Combining Wave Function Methods with Density Functional Theory for Excited States. <i>Chemical Reviews</i> , 2018, 118, 7249-7292.	23.0	166
9589	On the low magnetic field effect in radical pair reactions. <i>Journal of Chemical Physics</i> , 2018, 149, 034103.	1.2	27
9590	Can Popular DFT Approximations and Truncated Coupled Cluster Theory Describe the Potential Energy Surface of the Beryllium Dimer?. <i>Australian Journal of Chemistry</i> , 2018, 71, 804.	0.5	6
9591	Electronic structure and spectral properties of indole based fluorescent styryl dyes: Comprehensive study on linear and non-linear optical properties by DFT/TDDFT method. <i>Computational and Theoretical Chemistry</i> , 2018, 1139, 90-101.	1.1	18
9592	Lanthanide Complexes with Photochromic Organoboron Ligand: Synthesis and Luminescence Study. <i>Inorganic Chemistry</i> , 2018, 57, 10040-10049.	1.9	18
9593	Density functional theory studies on PVDF/ionic liquid composite systems. <i>Journal of Chemical Sciences</i> , 2018, 130, 1.	0.7	36
9594	Communication: Correct charge transfer in CT complexes from the Becke- TM 05 density functional. <i>Journal of Chemical Physics</i> , 2018, 148, 211101.	1.2	20
9595	Sigma-Holes in Battery Materials Using Iso-Electrostatic Potential Surfaces. <i>Crystals</i> , 2018, 8, 33.	1.0	6
9596	Monoclinic Paracetamol vs. Paracetamol-4,4'-Bipyridine Co-Crystal; What Is the Difference? A Charge Density Study. <i>Crystals</i> , 2018, 8, 46.	1.0	6
9597	Structures and electronic properties of halogenated Au(III) phthalocyanine AuPcX (X = Cl, Br): A Density Functional Theoretical Study. <i>Computational Materials Science</i> , 2018, 152, 262-267.	1.4	5
9598	Theoretical Studies on the Catalytic Cycle of Histidine Acid Phosphatases Revealing an Acid Proof Mechanism. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7530-7538.	1.2	5
9599	Quantum chemical study on the role of water in the reaction of singlet methoxysulfonyl nitrene CH ₃ OS(O)N ₂ . <i>Chemical Physics Letters</i> , 2018, 706, 548-552.	1.2	3
9600	An ab initio study on stacking and stability of TiAl ₃ phases. <i>Computational Materials Science</i> , 2018, 153, 309-314.	1.4	10
9601	Synthesis, Structural, Spectral, and Electrochemical Studies of Selenabenziporphyrin and Its Pd(II) Complex. <i>Inorganic Chemistry</i> , 2018, 57, 8956-8963.	1.9	15
9602	Syngas Production with a Highly-Robust Nickel(II) Homogeneous Electrocatalyst in a Water-Containing System. <i>ACS Catalysis</i> , 2018, 8, 7612-7620.	5.5	47
9603	Theoretical Studies of the Spin-Dependent Electronic Transport Properties in Ethynyl-Terminated Ferrocene Molecular Junctions. <i>Micromachines</i> , 2018, 9, 95.	1.4	5

#	ARTICLE	IF	CITATIONS
9604	Porphyrin Co(III)-Nitrene Radical Mediated Pathway for Synthesis of o-Aminoazobenzenes. <i>Molecules</i> , 2018, 23, 1052.	1.7	9
9605	Theoretical Investigations on Mechanisms and Pathways of C ₂ H ₅ O ₂ with BrO Reaction in the Atmosphere. <i>Molecules</i> , 2018, 23, 1268.	1.7	1
9606	Synthesis of Phlorin Analogues of Dithiacorrphycene and Their Use as Specific Chemodosimetric Sensors for Fe ³⁺ Ions. <i>Chemistry - an Asian Journal</i> , 2018, 13, 3040-3050.	1.7	5
9607	How Does a Heme Carbene Differ from Diatomic Ligated (NO, CO, and CN [−]) Analogues in the Axial Bond?. <i>Inorganic Chemistry</i> , 2018, 57, 8788-8795.	1.9	6
9608	Nonlinear-response properties in a simplified time-dependent density functional theory (sTD-DFT) framework: Evaluation of the first hyperpolarizability. <i>Journal of Chemical Physics</i> , 2018, 149, 024108.	1.2	41
9609	Theoretical estimation of the dissociation energy of CT states at the acenes/C ₆₀ interfaces using fragmental-based ALMO method. <i>Computational and Theoretical Chemistry</i> , 2018, 1140, 32-37.	1.1	2
9610	Synthesis, electronic structure and redox properties of the diruthenium sandwich complexes [Cp* ₂ Ru(1/4-C ₁₀ H ₈) ₂ RuCp*] _x (x = 0, 1+; Cp* = Tj) <i>ETQq0 0 0 rgBT /Overlock 10 Jf 50 502 T</i> 2018, 47, 11058-11069.	1.6	5
9611	Comparison of ZnO surface modification with gas-phase propiolic acid at high and medium vacuum conditions. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2018, 36, 041404.	0.9	3
9612	Helicenes Grafted with 1,1,4,4-Tetracyanobutadiene Moieties: Helical Push-Pull Systems with Strong Electronic Circular Dichroism and Two-Photon Absorption. <i>Chemistry - A European Journal</i> , 2018, 24, 14484-14494.	1.7	27
9613	Appraisal of 1-Butylimidazole-Derived Ionic Liquids as Anthelmintic Agents: An Experimental and In Silico Approach. <i>ChemistrySelect</i> , 2018, 3, 7518-7526.	0.7	4
9614	How Does Palladium-Amino Acid Cooperative Catalysis Enable Regio- and Stereoselective C(sp ³)-H Functionalization in Aldehydes and Ketones? A DFT Mechanistic Study. <i>ACS Catalysis</i> , 2018, 8, 7698-7709.	5.5	38
9615	Oxidopyrylium-Alkene [5 + 2] Cycloaddition Conjugate Addition Cascade (C ₃) Sequences: Scope, Limitation, and Computational Investigations. <i>Journal of Organic Chemistry</i> , 2018, 83, 9818-9838.	1.7	19
9616	Beyond the random phase approximation with a local exchange vertex. <i>Physical Review B</i> , 2018, 98, .	1.1	31
9617	[1,3]Thiazolo[3,2-b][1,2,4]triazol-7-ium salts: synthesis, properties and structural studies. <i>Heterocyclic Communications</i> , 2018, 24, 197-203.	0.6	15
9618	Noble gas hydrides in the triplet state: HNgCCO ⁺ (Ng = He, Ne, Ar, Kr, and Xe). <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20270-20279.	1.3	11
9619	Mechanistic Role of Two-State Reactivity in a Molecular MoS ₂ Edge-Site Analogue for Hydrogen Evolution Electrocatalysis. <i>Inorganic Chemistry</i> , 2018, 57, 9167-9174.	1.9	4
9620	Resolving the excited state relaxation dynamics of guanosine monomers and hydrogen-bonded homodimers in chloroform solution. <i>Chemical Physics</i> , 2018, 515, 480-492.	0.9	2
9621	ONIOM studies on thermally activated delayed fluorescence of copper(I) dimers in crystal. <i>Chemical Physics</i> , 2018, 515, 692-703.	0.9	10

#	ARTICLE	IF	CITATIONS
9622	Reactions of the Ni(0) Compound Ni(PPh ₃) ₄ with Unactivated Alkyl Halides: Oxidative Addition Reactions Involving Radical Processes and Nickel(I) Intermediates. <i>Organometallics</i> , 2018, 37, 2450-2467.	1.1	38
9623	New Ru(II) photocages operative with near-IR light: new platform for drug delivery in the PDT window. <i>Chemical Science</i> , 2018, 9, 6711-6720.	3.7	71
9624	Time-dependent generalized Kohn–Sham theory. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	75
9625	The influence of the structural variations of the fused electron rich-electron deficient unit in the Ī-spacer of A-D-Ī-D-A organic dyes on the efficiency of dye-sensitized solar cells: A computational study. <i>Organic Electronics</i> , 2018, 62, 43-55.	1.4	13
9626	Structure and kinetics of water in highly confined conditions: A molecular dynamics simulation study. <i>Journal of Molecular Liquids</i> , 2018, 268, 625-636.	2.3	32
9627	Design and Emissive Features of Ionic White-Light Fluorophore. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18615-18620.	1.5	14
9628	Hydrolysis and substitution effects on the optical properties of coumarin derivatives studied by vibrational spectroscopy and DFT calculation. <i>Journal of Molecular Structure</i> , 2018, 1168, 65-72.	1.8	10
9629	Photoinduced intramolecular charge transfer in a cross-conjugated push–pull enediyne: implications toward photoreaction. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14889-14898.	1.3	8
9630	Thermoelectric Performance of an Open-Shell Donor–Acceptor Conjugated Polymer Doped with a Radical-Containing Small Molecule. <i>Macromolecules</i> , 2018, 51, 3886-3894.	2.2	51
9631	Novel Phenothiazine–oxide Based Push–Pull Molecules: Synthesis and Fine-Tuning of Electronic, Optical and Thermal Properties. <i>ChemistrySelect</i> , 2018, 3, 5073-5081.	0.7	9
9632	Experimental and quantum chemical studies of functionalized tetrahydropyridines as corrosion inhibitors for mild steel in 1 M hydrochloric acid. <i>Results in Physics</i> , 2018, 9, 1481-1493.	2.0	78
9633	Theoretical study on the effective dehydrochlorination of 1,2-dichloroethane catalyzed by tetraalkylphosphonium chlorides: electrostatically controlled reactivity. <i>New Journal of Chemistry</i> , 2018, 42, 10084-10091.	1.4	2
9635	Hydrogen Evolution Reactions Catalyzed by a Bis(thiosemicarbazone) Cobalt Complex: An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2018, 24, 8779-8786.	1.7	50
9636	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4756-4767.	1.1	41
9637	Porous Hexagonal Boron Nitride Sheets: Effect of Hydroxyl and Secondary Amino Groups on Photocatalytic Hydrogen Evolution. <i>ACS Applied Nano Materials</i> , 2018, 1, 4566-4575.	2.4	119
9638	Twist and Return–Induced Ring Strain Triggers Quick Relaxation of a (Z)-Stabilized Cyclobisazobenzene. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4776-4781.	2.1	17
9639	Modulating the DNA cleavage ability of copper(II) Schiff bases through ternary complex formation. <i>New Journal of Chemistry</i> , 2018, 42, 15170-15183.	1.4	12
9640	First-principles study of efficient phenothiazine-based Ī organic sensitizers with various spacers for DSSCs. <i>Journal of Computational Electronics</i> , 2018, 17, 1410-1420.	1.3	35

#	ARTICLE	IF	CITATIONS
9641	A density functional theory investigation of the fragmentation mechanism of deprotonated asparagine. <i>Computational and Theoretical Chemistry</i> , 2018, 1141, 45-52.	1.1	2
9642	The mechanism of NO and N ₂ O decomposition catalyzed by short-distance Cu(I) pairs in Cu-ZSM-5: A DFT study on the possible role of NO and NO ₂ in the [Cu O Cu] ₂ ⁺ active site reduction. <i>Journal of Catalysis</i> , 2018, 366, 189-201.	3.1	10
9643	Robust Periodic Fock Exchange with Atom-Centered Gaussian Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4567-4580.	2.3	17
9644	A molecular mechanism for the enzymatic methylation of nitrogen atoms within peptide bonds. <i>Science Advances</i> , 2018, 4, eaat2720.	4.7	48
9645	Synthesis, Characterization, and Nanomaterials Generated from 6,6'-bis(2-hydroxyethyl)azanediylobis(methylene)bis(2,4-di- <i>tert</i> -butylphenol) Modified Group 4 Metal Alkoxides. <i>Inorganic Chemistry</i> , 2018, 57, 11264-11274.	1.9	8
9646	Theoretical study of the decomposition mechanism of SF ₆ /Cu gas mixtures. <i>Journal Physics D: Applied Physics</i> , 2018, 51, 425202.	1.3	8
9647	Efficiency difference between furan- and thiophene-based D&A dyes in DSSCs explained by theoretical calculations. <i>RSC Advances</i> , 2018, 8, 29917-29923.	1.7	10
9648	DFT/TD-DFT calculations of the electronic and optical properties of bis-N,N-dimethylaniline-based dyes for use in dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 367, 332-346.	2.0	17
9649	Extended First Hyperpolarizability of Quasi-Octupolar Molecules by Halogenated Methylation: Whether the Iodine Atom is the Best Choice. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21548-21556.	1.5	30
9650	Catalytic Enantioselective [10+4] Cycloadditions. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 13182-13186.	7.2	42
9651	Explicit Aqueous Solvation Treatment of Epinephrine from Car Parrinello Molecular Dynamics: Effect of Hydrogen Bonding on the Electronic Absorption Spectrum. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8439-8450.	1.2	7
9652	How well can density functional theory and pair-density functional theory predict the correct atomic charges for dissociation and accurate dissociation energetics of ionic bonds?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23072-23078.	1.3	11
9653	Reactions of N-alkenyl Thioureas with p-alkoxyphenyltellurium Trichlorides. <i>Journal of Heterocyclic Chemistry</i> , 2018, 55, 2284-2290.	1.4	14
9654	Identification of a new high-molecular-weight Fe ^{III} citrate species at low citrate-to-Fe molar ratios: Impact on arsenic removal with ferric hydroxide. <i>Chemosphere</i> , 2018, 212, 50-55.	4.2	3
9655	Divergent Diels-Alder Reactions in the Biosynthesis and Synthesis of Endiandric-Type Tetracycles: A Computational Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 10941-10947.	1.7	6
9656	Catalytic Enantioselective [10+4] Cycloadditions. <i>Angewandte Chemie</i> , 2018, 130, 13366-13370.	1.6	10
9657	Light induced DNA-functionalized TiO ₂ nanocrystalline interface: Theoretical and experimental insights towards DNA damage detection. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2018, 188, 159-176.	1.7	18
9658	Mononuclear thorium halide clusters ThX ₄ (X = F, Cl): gas-phase hydrolysis reactions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21184-21193.	1.3	6

#	ARTICLE	IF	CITATIONS
9659	Electronic stopping power from time-dependent density-functional theory in Gaussian basis. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	28
9660	Theoretical Prediction of Structural, Electronic, and Magnetic Properties of Rh ₂ Y In (Y = Nd, Sm) Full-Heusler Alloys. <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 3091-3095.	0.8	3
9661	Doped aluminum nanocones as an efficient electron field emitter: A first-principles investigation. <i>Inorganic Chemistry Communication</i> , 2018, 96, 5-12.	1.8	16
9662	Assessment of Density Functional Approximations for Highly Correlated Oxides: The Case of CeO ₂ and Ce ₂ O ₃ . <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4914-4927.	2.3	27
9663	Kinetics of the Reaction of the Cyclopentadienyl Radical with Nitrogen Dioxide. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6978-6984.	1.1	0
9664	DFT Studies of Perfluorosulfonic Acid Ionomer Degradation in Fuel Cells. <i>Journal of Physical Chemistry C</i> , 2018, 122, 20135-20143.	1.5	15
9665	On the challenge to improve the density response with unusual gradient approximations. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	4
9666	Electronic structure of isomeric graphene nanoflakes. <i>Computational and Theoretical Chemistry</i> , 2018, 1140, 125-133.	1.1	8
9667	Theoretical investigation of structures and electromagnetic properties of double-electron oxidized ring-expanded base pairs. <i>Chemical Physics Letters</i> , 2018, 707, 86-92.	1.2	2
9668	Redox Innocence of Re(I) in Electrochemical CO ₂ Reduction Catalyzed by Nanographene-Re Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 10548-10556.	1.9	11
9669	Fluorescent meso-benzyl curcuminoid boron complex: Synthesis, photophysics, DFT and NLO study. <i>Optical Materials</i> , 2018, 84, 786-794.	1.7	17
9670	Evaluating Nucleophile Byproduct Formation during Phosphine- and Amine-Promoted Thiol-Methyl Acrylate Reactions. <i>Journal of Organic Chemistry</i> , 2018, 83, 10370-10382.	1.7	9
9671	Complexation of NpO ₂ ⁺ with Amine-Functionalized Diacetamide Ligands in Aqueous Solution: Thermodynamic, Structural, and Computational Studies. <i>Inorganic Chemistry</i> , 2018, 57, 6965-6972.	1.9	10
9672	Can Formamide Be Formed on Interstellar Ice? An Atomistic Perspective. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 720-734.	1.2	83
9673	An experimental and theoretical study on the kinetics of the reaction between 4-hydroxyhexanone CH ₃ CH ₂ C(O)CH(OH)CH ₂ CH ₂ CH ₃ and OH radicals. <i>International Journal of Chemical Kinetics</i> , 2018, 50, 556-567.	1.0	5
9674	Studies of fluorine auxochrome in C ₉ -fluorenyl anthracenes on optoelectronic property for blue electroluminescent materials. <i>Dyes and Pigments</i> , 2018, 158, 420-427.	2.0	8
9675	How fine-tuned for energy transfer is the environmental noise produced by proteins around biological chromophores?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17279-17288.	1.3	7
9676	Beyond the Woodward-Hoffman Rules: What Controls Reactivity in Eliminative Aromatic Ring-Forming Reactions?. <i>Australian Journal of Chemistry</i> , 2018, 71, 249.	0.5	3

#	ARTICLE	IF	CITATIONS
9677	Oxidation of Cymantrene Analogues of Ferrocifen: Electrochemical, Spectroscopic, and Computational Studies of the Parent Complex 1,1'-Diphenyl-2-cymantrenylbutene. <i>Organometallics</i> , 2018, 37, 1910-1918.	1.1	6
9678	Efficient and Linear-Scaling Seminumerical Method for Local Hybrid Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3451-3458.	2.3	30
9679	Synthesis and luminescent properties of novel organic luminescent materials based on carbazole derivatives. <i>Chemical Papers</i> , 2018, 72, 2955-2963.	1.0	2
9680	Linear correlation between DSSC efficiency, intramolecular charge transfer characteristics, and NLO properties – DFT approach. <i>Computational and Theoretical Chemistry</i> , 2018, 1138, 75-83.	1.1	56
9681	Density functional study of half-metallicity and spin polarization in Fe _{1-x} T _x S ₂ with T = Mn, Ni. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 305501.	0.7	3
9682	A theoretical study of a series of water-soluble triphenylamine photosensitizers for two-photon photodynamic therapy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 203, 229-235.	2.0	3
9683	Quantum-Chemical Ab Initio Calculations on Inda- and Thallabenzene (C ₅ H ₅ In and C ₅ H ₅ Tl) and their Structural Isomers 1,5-C ₅ H ₅ In and 1,5-C ₅ H ₅ Tl. <i>Australian Journal of Chemistry</i> , 2018, 71, 102.	0.5	1
9684	Accuracy of TD-DFT Geometries: A Fresh Look. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3715-3727.	2.3	74
9685	Theoretical design of porphyrin sensitizers with different acceptors for application in dye-sensitized solar cells. <i>RSC Advances</i> , 2018, 8, 19804-19810.	1.7	10
9686	Free Energy Analyses for the ATP Hydrolysis in Aqueous Solution by Large-Scale QM/MM Simulations Combined with a Theory of Solutions. , 2018, , 3-23.		0
9687	Exciton energy transfer in organic light emitting diodes with thermally activated delayed fluorescence dopants. <i>Journal of Materials Chemistry C</i> , 2018, 6, 6860-6868.	2.7	12
9688	Computational Study on Gold-Catalyzed Cascade Reactions of 1,4-Diynes and Pyrroles: Mechanism, Regioselectivity, Role of Catalyst, and Effects of Substituent and Solvent. <i>Organometallics</i> , 2018, 37, 1927-1936.	1.1	15
9689	Relaxation of photoexcitations in polaron-induced magnetic microstructures. <i>Physical Review B</i> , 2018, 97, .	1.1	6
9690	Boron Centres Allow Design, Control and Systematic Tuning of Neutral Homoaromatics for Functionalization Purposes. <i>ChemPhysChem</i> , 2018, 19, 2525-2533.	1.0	0
9691	Simulating X-ray Spectroscopies and Calculating Core-Excited States of Molecules. <i>Chemical Reviews</i> , 2018, 118, 7208-7248.	23.0	214
9692	Charge Transfer Excitations with Range Separated Functionals Using Improved Virtual Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3667-3676.	2.3	3
9693	D ² -benzo[1,2,3]triazole derivatives as p-type semiconductors in organic field-effect transistors. <i>RSC Advances</i> , 2018, 8, 21879-21888.	1.7	13
9694	Neural-network Kohn-Sham exchange-correlation potential and its out-of-training transferability. <i>Journal of Chemical Physics</i> , 2018, 148, 241737.	1.2	60

#	ARTICLE	IF	CITATIONS
9695	The computational study of bridge effect in D- π -A photosensitive dyes, based on triphenylamine. IOP Conference Series: Earth and Environmental Science, 2018, 161, 012021.	0.2	4
9696	Electronic structure and large second-order non-linear optical property of COT derivatives – a theoretical exploration. Physical Chemistry Chemical Physics, 2018, 20, 18744-18755.	1.3	6
9697	Molecular design towards suppressing electron recombination and enhancing the light-absorbing ability of dyes for use in sensitized solar cells: a theoretical investigation. New Journal of Chemistry, 2018, 42, 12891-12899.	1.4	10
9698	Molecular docking, molecular modeling, vibrational and biological studies of some new heterocyclic \pm -aminophosphonates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 206, 78-88.	2.0	27
9699	Toward a better understanding of the interaction between somatostatin receptor 2 and its ligands: a structural characterization study using molecular dynamics and conceptual density functional theory. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3081-3102.	2.0	9
9700	Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1378.	6.2	95
9701	Spectral Faraday rotation in tripyridinium bis[tetrachloroferrate(III)] chloride molecular magnet at room temperature due to electronic transition. Journal of Magnetism and Magnetic Materials, 2019, 469, 13-18.	1.0	1
9702	PySCF-NAO: An efficient and flexible implementation of linear response time-dependent density functional theory with numerical atomic orbitals. Computer Physics Communications, 2019, 236, 188-204.	3.0	8
9703	Case study of 2-vinylpyridine: Quantitative assessment of the intramolecular C-H \cdots N hydrogen bond energy and its contribution to the one-bond ^{13}C coupling constant. Journal of Molecular Structure, 2019, 1176, 73-85.	1.8	9
9704	Spectroscopic investigation and computational studies on the interaction of Acriflavine with various estrogens. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 206, 622-629.	2.0	5
9705	Intramolecular hydrogen bonding patterns, conformational preferences and molecular properties of dimeric acylphloroglucinols: An ab initio and DFT study. Journal of Molecular Structure, 2019, 1176, 488-500.	1.8	15
9706	Electronic Properties of Realistic Anatase TiO_2 Nanoparticles from GW Calculations on a Gaussian and Plane Waves Scheme. Journal of Chemical Theory and Computation, 2019, 15, 5024-5030.	2.3	7
9707	Modeling of Spin Crossover in Iron(II) Complexes with N_4S_2 Coordination. Journal of Physical Chemistry C, 2019, 123, 19984-19990.	1.5	5
9708	Isolation and Computational Studies of a Series of Terphenyl Substituted Diplumbynes with Ligand Dependent Lead–Lead Multiple-Bonding Character. Journal of the American Chemical Society, 2019, 141, 14370-14383.	6.6	21
9709	Lewis Acid Transition-Metal-Catalyzed Hydrogen Activation: Structures, Mechanisms, and Reactivities. Chemistry - A European Journal, 2019, 25, 13785-13798.	1.7	13
9710	Synthesis and Characterization of Some BODIPY-based Substituted Salicylaldehyde Schiff Bases. Journal of Heterocyclic Chemistry, 2019, 56, 2499-2507.	1.4	5
9711	Fate of oxygen species from O_2 activation at dimetal cofactors in an oxidase enzyme revealed by ^{57}Fe nuclear resonance X-ray scattering and quantum chemistry. Biochimica Et Biophysica Acta - Bioenergetics, 2019, 1860, 148060.	0.5	1
9712	Bis(4,4'-biphenyl Ring Embedded Octaphyrin with Three Distinct Conformational Structures. Chemistry - A European Journal, 2019, 25, 12911-12915.	1.7	14

#	ARTICLE	IF	CITATIONS
9713	Effects of complexation with a metal ion on the intramolecular hydrogen bonds in acylphloroglucinols. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	1
9715	Excited-State Triplet Equilibria in a Series of Re(I)-Naphthalimide Bichromophores. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7611-7627.	1.2	23
9716	Conformational Changes as Driving Force for Phase Recognition: The Case of Laurdan. <i>Langmuir</i> , 2019, 35, 11471-11481.	1.6	21
9717	Theoretical Study of the Mechanisms of Two Copper Water Oxidation Electrocatalysts with Bipyridine Ligands. <i>ACS Catalysis</i> , 2019, 9, 8798-8809.	5.5	9
9718	Steric control of dioxygen activation pathways for MnII complexes supported by pentadentate, amide-containing ligands. <i>Dalton Transactions</i> , 2019, 48, 13034-13045.	1.6	10
9719	Chemical and Morphological Origins of Improved Ion Conductivity in Perfluoro Ionene Chain Extended Ionomers. <i>Journal of the American Chemical Society</i> , 2019, 141, 13547-13561.	6.6	34
9720	Germacrone Derivatives as new Insecticidal and Acaricidal Compounds: A Structure-Activity Relationship. <i>Molecules</i> , 2019, 24, 2898.	1.7	4
9721	Synthesis, Density Functional Theory Band Structure Calculations, Optical, and Photoelectrical Characterizations of the Novel (9-Bromo-3-cyano-5-oxo-1,5-dihydro-2H-chromeno[4,3-b]) Tj ETQ ₁ 1 0.784314 rgBT	1.1	0
9722	Mechanistic insights into ring cleavage of hydroquinone by PnpCD from quantum mechanical/molecular mechanical calculations. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 8194-8205.	1.5	5
9723	Statistically representative databases for density functional theory <i>via</i> data science. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19092-19103.	1.3	20
9724	Unraveling the marked differences of the phosphorescence efficiencies of blue-emitting iridium complexes with isomerized phenyltriazole ligands. <i>Inorganic Chemistry Frontiers</i> , 2019, 6, 2776-2787.	3.0	5
9725	Rational magnetic modification of <i>N,N</i> -dioxidized pyrazine ring expanded adenine and thymine: a diradical character induced by base pairing and double protonation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20095-20106.	1.3	3
9726	Femtosecond Stimulated Raman Scattering from Triplet Electronic States: Experimental and Theoretical Study of Resonance Enhancements. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7720-7732.	1.1	9
9727	Theoretical UV-Vis spectra of tetracationic porphyrin: effects of environment on electronic spectral properties. <i>Journal of Molecular Modeling</i> , 2019, 25, 264.	0.8	5
9728	Alkylation of 2-oxo(thioxo)-thieno[2,3-d]pyrimidine-4-ones: Experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2019, 1198, 126858.	1.8	16
9729	Computational Studies of Adsorption of Toxic Molecules and Anions on the Surface of Doped and Functionalized Carbon Nanotubes. <i>Springer Proceedings in Physics</i> , 2019, , 305-340.	0.1	2
9730	Beyond Density Functional Theory: The Multiconfigurational Approach To Model Heterogeneous Catalysis. <i>ACS Catalysis</i> , 2019, 9, 8481-8502.	5.5	75
9731	Decay pathways for protonated and deprotonated adenine molecules. <i>Journal of Chemical Physics</i> , 2019, 151, 044306.	1.2	0

#	ARTICLE	IF	CITATIONS
9732	Dispersion XDM with Hybrid Functionals: Delocalization Error and Halogen Bonding in Molecular Crystals. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4933-4944.	2.3	22
9733	M11plus: A Range-Separated Hybrid Meta Functional with Both Local and Rung-3.5 Correlation Terms and High Across-the-Board Accuracy for Chemical Applications. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4804-4815.	2.3	24
9734	Calculating rate constants for intersystem crossing and internal conversion in the Franck-Condon and Herzberg-Teller approximations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18495-18500.	1.3	38
9735	On combining the conductor-like screening model and optimally tuned range-separated hybrid density functionals. <i>Journal of Chemical Physics</i> , 2019, 150, 174117.	1.2	9
9736	The sensitization effect and microscopic essence of different additives on the electronic structure of nanocrystalline TiO ₂ in dye-sensitized solar cell. <i>Solar Energy</i> , 2019, 189, 372-384.	2.9	2
9737	Toward a Quantum-Chemical Benchmark Set for Enzymatically Catalyzed Reactions: Important Steps and Insights. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7057-7074.	1.1	19
9738	Kinetic hydricity of silane hydrides in the gas phase. <i>Chemical Science</i> , 2019, 10, 8002-8008.	3.7	5
9739	Ab initio and density functional theory study of the electronic structure of rhenium complexes with noninnocent dioxolene ligands: Localized vs delocalized valence states. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e26018.	1.0	0
9740	Tridentate diarylamido-based pincer complexes of nickel and palladium: sidearm effects in the polymerization of norbornene. <i>Dalton Transactions</i> , 2019, 48, 12219-12227.	1.6	12
9741	Tautomerism in Azo and Azomethyne Dyes: When and If Theory Meets Experiment. <i>Molecules</i> , 2019, 24, 2252.	1.7	31
9742	A Density-Functional Theory of CO ₂ Interaction with a Hafnium-Titanium Nanocluster. <i>Russian Journal of Inorganic Chemistry</i> , 2019, 64, 88-97.	0.3	0
9743	Thermal Decomposition of B(C ₆ F ₅) ₃ ·Py Complex. <i>Russian Journal of General Chemistry</i> , 2019, 89, 1162-1168.	0.3	7
9744	Ï%B2PLYP and Ï%B2GPPLYP: The First Two Double-Hybrid Density Functionals with Long-Range Correction Optimized for Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4735-4744.	2.3	107
9745	Machine-learned electron correlation model based on correlation energy density at complete basis set limit. <i>Journal of Chemical Physics</i> , 2019, 151, 024104.	1.2	24
9746	Electronic structure and second-order nonlinear optical property of chiral peropyrenes. <i>Journal of Molecular Modeling</i> , 2019, 25, 220.	0.8	1
9747	Dissociative ionization dynamics of dielectric gas C ₃ F ₇ CN. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16451-16458.	1.3	21
9748	Role of the Photosystem II as an Environment in the Oxidation Free Energy of the Mn Cluster from S ₁ to S ₂ . <i>Journal of Physical Chemistry B</i> , 2019, 123, 7081-7091.	1.2	5
9749	Theoretical and experimental investigation on the electrochemical properties, structural and spectroscopic parameters of 6,7-dihydroxy-9-thia-1,4a-diaza fluoren-2-one (DTDFO). <i>Journal of Sulfur Chemistry</i> , 2019, 40, 598-613.	1.0	0

#	ARTICLE	IF	CITATIONS
9750	Large Increase in External Quantum Efficiency by Dihedral Angle Tuning in a Skyâ€Blue Thermally Activated Delayed Fluorescence Emitter. <i>Advanced Optical Materials</i> , 2019, 7, 1900476.	3.6	25
9751	Elucidating the Doping Effect on the Electronic Structure of Thiolateâ€Protected Silver Superatoms by Photoelectron Spectroscopy. <i>Angewandte Chemie</i> , 2019, 131, 11763-11767.	1.6	5
9752	Methane Activation by (n=0, 1, 2; m= 1, 2): Reactivity Parameters, Electronic Properties and Binding Energy Analysis. <i>ChemistrySelect</i> , 2019, 4, 7912-7921.	0.7	0
9753	Membrane-specific spin trap, 5-dodecylcarbamoyl-5- <i>N</i> -dodecylacetamide-1-pyroline- <i>N</i> -oxide (diC ₁₂ PO): theoretical, bioorthogonal fluorescence imaging and EPR studies. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 7694-7705.	1.5	5
9754	Geometry and Electronic Structure of the P-Cluster in Nitrogenase Studied by Combined Quantum Mechanical and Molecular Mechanical Calculations and Quantum Refinement. <i>Inorganic Chemistry</i> , 2019, 58, 9672-9690.	1.9	20
9755	Theoretical investigation of the chiral transition of serine and the roles of water, hydroxyl radical and hydroxide ion. <i>New Journal of Chemistry</i> , 2019, 43, 12340-12350.	1.4	1
9756	Low-Frequency Raman Spectroscopic Study on Compression-Induced Destabilization in Melt-Quenched Amorphous Celecoxib. <i>Molecular Pharmaceutics</i> , 2019, 16, 3678-3686.	2.3	25
9757	Structural and Thermoelectric Properties of Solidâ€Liquid In ₄ Se ₃ -In Composite. <i>Journal of Electronic Materials</i> , 2019, 48, 5418-5427.	1.0	7
9758	Conical Intersections in Organic Molecules: Benchmarking Mixed-Reference Spinâ€Flip Time-Dependent DFT (MRSF-TD-DFT) vs Spinâ€Flip TD-DFT. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6455-6462.	1.1	35
9759	Theoretical treatment of semiconductor heterojunctions for photocatalysis: the WO ₃ /BiVO ₄ interface. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 434001.	0.7	16
9760	A scaled CIS(D) based method for the calculation of valence and core electron ionization energies. <i>Journal of Chemical Physics</i> , 2019, 151, 034104.	1.2	10
9761	The Potential Application of BAs for a Gas Sensor for Detecting SO ₂ Gas Molecule: a DFT Study. <i>Nanoscale Research Letters</i> , 2019, 14, 133.	3.1	24
9762	Ortho â€Quinone Methide Driven Synthesis of New O , N â€or N , N â€Heterocycles. <i>ChemistryOpen</i> , 2019, 8, 961-971.	0.9	5
9763	Syntheses, Crystal Structures and Experimental/Theoretical Magnetic Properties of Two Butterfly Ni II 2 Y III 2 Compounds. <i>ChemistrySelect</i> , 2019, 4, 8074-8081.	0.7	0
9764	How To Extract Quantitative Information on Electronic Transitions from the Density Functional Theory â€Black Boxâ€. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4915-4923.	2.3	9
9765	Synthesis and Studies of Strained Fluorenophyrins. <i>Journal of Organic Chemistry</i> , 2019, 84, 10321-10327.	1.7	15
9766	NHC-catalyzed green synthesis of functionalized chromones: DFT mechanistic insights and <i>in vitro</i> activities in cancer cells. <i>New Journal of Chemistry</i> , 2019, 43, 13509-13525.	1.4	16
9767	Design and photoelectric properties of D-A-ËA carbazole dyes with different Ë-spacers and acceptors for use in solar cells: a DFT and TD-DFT investigation. <i>Journal of Molecular Modeling</i> , 2019, 25, 249.	0.8	5

#	ARTICLE	IF	CITATIONS
9768	Optimal transport and colossal ionic mechano-conductance in graphene crown ethers. <i>Science Advances</i> , 2019, 5, eaaw5478.	4.7	37
9769	SO ₂ gas adsorption on the transition metal (Pd, Ag, Au and Pt) -doped monolayer MoSe ₂ : A first-principles study. <i>Chemical Physics Letters</i> , 2019, 733, 136631.	1.2	21
9770	Synthesis and in silico characterization of artificially phosphorylated glycosaminoglycans. <i>Journal of Molecular Structure</i> , 2019, 1197, 401-416.	1.8	8
9771	Assessment of BODIPY ⁺ Oxasmaragdyrin Dyads for Dye-Sensitized Solar Cells: Aromaticity, Photosensitization Capability, and Charge Transport. <i>Journal of Physical Chemistry C</i> , 2019, 123, 19362-19375.	1.5	15
9772	Enhanced intramolecular charge transfer of organic dyes containing hydantoin donor: A DFT study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 383, 111979.	2.0	11
9773	Bootstrap Embedding for Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4497-4506.	2.3	22
9774	An Ab initio study of double-electron oxidized base pairs with diradical character through ring-expansion modification. <i>Computational and Theoretical Chemistry</i> , 2019, 1164, 112539.	1.1	0
9775	Experimental and theoretical exploration of sensing and magnetic properties of a triply bridged dicopper(II) complex: The first discrete metal complex to sense picric acid in pure water. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 383, 111987.	2.0	11
9776	Extension and acceleration of relativistic density functional theory based on transformed density operator. <i>Journal of Chemical Physics</i> , 2019, 150, 164104.	1.2	11
9777	Planarity of ethylene/linear polyene analogues focused on π -electron holding ability of the components. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e26029.	1.0	2
9779	Inter and intra-phase conformerism in two calix [4]arenes. <i>Journal of Molecular Structure</i> , 2019, 1198, 126849.	1.8	0
9780	Reduction in Coordination Number of Eu(III) on Complexation with Pyrazine Mono- and Di-Carboxylates in Aqueous Medium. <i>Inorganic Chemistry</i> , 2019, 58, 11180-11194.	1.9	20
9781	Reaction mechanism of nucleoside 2'-deoxyribosyltransferases: free-energy landscape supports an oxocarbenium ion as the reaction intermediate. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 7891-7899.	1.5	10
9782	Oxygen Reduction Reaction Mechanisms on Heteroatom-Doped Single-Walled Carbon Nanotube Catalysts: Insights from a Theoretical Study. <i>Journal of the Electrochemical Society</i> , 2019, 166, F670-F678.	1.3	15
9783	Using Ultrafast X-ray Spectroscopy To Address Questions in Ligand-Field Theory: The Excited State Spin and Structure of [Fe(dcpp) ₂] ²⁺ . <i>Inorganic Chemistry</i> , 2019, 58, 9341-9350.	1.9	29
9784	Highly Electron-Deficient Pyridinium-Nitrones for Rapid and Tunable Inverse-Electron-Demand Strain-Promoted Alkyne-Nitrone Cycloaddition. <i>Organic Letters</i> , 2019, 21, 5547-5551.	2.4	11
9785	Stereoselective Excited-State Isomerization and Decay Paths in <i>cis</i> -Cyclobiazobenzene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6144-6151.	1.1	5
9786	A Benchmark of Density Functional Approximations For Thermochemistry and Kinetics of Hydride Reductions of Cyclohexanones. <i>ChemistryOpen</i> , 2019, 8, 788-806.	0.9	7

#	ARTICLE	IF	CITATIONS
9787	Stereo-inversion in the diastereoselective acylation of benzoxazine derivatives with 2-aryloxypropionyl chlorides. <i>Russian Chemical Bulletin</i> , 2019, 68, 1257-1263.	0.4	5
9788	Structural and photophysical studies of triphenylamine-based nonlinear optical dyes: effects of π -linker moieties on the D- π -A structure. <i>Comptes Rendus Chimie</i> , 2019, 22, 373-385.	0.2	10
9789	Coupled Cluster Theory with Induced Dipole Polarizable Embedding for Ground and Excited States. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4485-4496.	2.3	13
9790	Contribution of substrate reorganization energies of electron transfer to laccase activity. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15805-15814.	1.3	9
9791	Theoretical insights into inorganic-organic intercalation products of the layered perovskite HLaNb_2O_7 : perspectives for hybrid proton conductors. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16647-16657.	1.3	3
9792	On the influence of water on fragmentation of the amino acid L-threonine. <i>Open Physics</i> , 2019, 17, 250-262.	0.8	0
9793	Cross-Comparisons between Experiment, TD-DFT, CC, and ADC for Transition Energies. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4581-4590.	2.3	58
9794	Meso-Fused Carbatriphyrins(2.1.1) and Its Organo Phosphorus(V) Complex. <i>Journal of Organic Chemistry</i> , 2019, 84, 9067-9074.	1.7	20
9795	DFT study on the effect of proximal residues on the <i>Mycobacterium tuberculosis</i> catalase-peroxidase (katG) heme compound I intermediate and its bonding interaction with isoniazid. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16515-16525.	1.3	7
9796	Feasibility of a high stable PbTe:In semiconductor for thermoelectric energy applications. <i>Journal of Applied Physics</i> , 2019, 125, .	1.1	42
9797	Étude structurale des systèmes dissymétriques de structure D- π -A à base de thiopyrazine destinés aux cellules solaires organiques de type « bulk heterojunction » (BHJ). <i>Canadian Journal of Chemistry</i> , 2019, 97, 745-755.	0.6	1
9798	Optimizing linear polymer affinity agent properties for surface-enhanced Raman scattering detection of aflatoxin B1. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 1019-1031.	1.7	17
9799	Chemical Kinetics of Hydrogen Atom Abstraction from Propargyl Sites by Hydrogen and Hydroxy Radicals. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3227.	1.8	6
9800	Octacarbonyl Ion Complexes of Actinides $[\text{An}(\text{CO})_8]^{+/\sim}$ (An=Th, U) and the Role of f Orbitals in Metal-Ligand Bonding. <i>Chemistry - A European Journal</i> , 2019, 25, 11772-11784.	1.7	38
9801	Ligand-Dependent Energetics for Dehydrogenation: Implications in Li-Ion Battery Electrolyte Stability and Selective Oxidation Catalysis of Hydrogen-Containing Molecules. <i>Chemistry of Materials</i> , 2019, 31, 5464-5474.	3.2	28
9802	Nuclear Motion in the Intramolecular Dihydrogen-Bound Regime of an Aminoborane Complex. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6547-6563.	1.1	0
9803	Hopanoids Like Sterols Form Compact but Fluid Films. <i>Langmuir</i> , 2019, 35, 9848-9857.	1.6	16
9804	Gas-Phase and Ionic Liquid Experimental and Computational Studies of Imidazole Acidity and Carbon Dioxide Capture. <i>Journal of Organic Chemistry</i> , 2019, 84, 14593-14601.	1.7	10

#	ARTICLE	IF	CITATIONS
9805	Investigation of the Absorption Cross Section of Phenyl Radical and Its Kinetics with Methanol in the Gas Phase Using Cavity Ring-Down Spectroscopy and Theoretical Methodologies. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9682-9692.	1.1	11
9806	Application of Multifunctional X-Doped Sumanene (X= Si, Ge, O, S and Se) for Concave-Convex Supramolecular Assembly with C ₆₀ and Their Nonlinear Optical Properties. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27811-27822.	1.5	9
9807	Effective one-particle energies from generalized Kohn-Sham random phase approximation: A direct approach for computing and analyzing core ionization energies. <i>Journal of Chemical Physics</i> , 2019, 151, 134106.	1.2	16
9808	Computational Exploration of Chiral Iron Porphyrin-Catalyzed Asymmetric Hydroxylation of Ethylbenzene Where Stereoselectivity Arises from π - π Stacking Interaction. <i>Journal of Organic Chemistry</i> , 2019, 84, 13755-13763.	1.7	10
9809	Machine Learning the Physical Nonlocal Exchange-Correlation Functional of Density-Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6425-6431.	2.1	62
9810	Computational Investigation of Drug Phototoxicity: Photosafety Assessment, Photo-Toxophore Identification, and Machine Learning. <i>Chemical Research in Toxicology</i> , 2019, 32, 2338-2352.	1.7	27
9811	Identifying Adhesion Properties at Si/Polymer Interfaces with ReaxFF. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27036-27047.	1.5	10
9812	Tailoring of Bandgap to Tune the Optical Properties of Ga _{1-x} Al _x Y (Y = As, Sb) for Solar Cell Applications by Density Functional Theory Approach. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2019, 74, 1131-1138.	0.7	3
9813	Activation of the Aromatic Core of 3,3'-bis(2-(pyridine-2,6-diylbis(1 <i>H</i> -1,2,3-triazole-4,1-diyl))bis(propan-1-ol)) Effects on Extraction Performance, Stability Constants, and Basicity. <i>Inorganic Chemistry</i> , 2019, 58, 14642-14651.	1.9	23
9814	Benchmark study of the linear and nonlinear optical polarizabilities in proto-type NLO molecule of <i>para</i> -nitroaniline. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950030.	1.8	74
9816	Influence of UV stabilizers on the weathering of PETG and PCTT films. <i>Journal of Applied Polymer Science</i> , 2019, 136, 48198.	1.3	8
9817	Mechanistic Insights on the Functionalization of CO ₂ with Amines and Hydrosilanes Catalyzed by a Zwitterionic Iridium Carboxylate-Functionalized Bis-NHC Catalyst. <i>ChemCatChem</i> , 2019, 11, 5524-5535.	1.8	20
9818	Effect of ring size on photoisomerization properties of stiff stilbene macrocycles. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 2408-2418.	1.3	7
9819	Light driven deracemization enabled by excited state electron transfer. <i>Science</i> , 2019, 366, 364-369.	6.0	188
9820	Assessing density functional theory in real-time and real-space as a tool for studying bacteriochlorophylls and the light-harvesting complex 2. <i>Journal of Chemical Physics</i> , 2019, 151, 134114.	1.2	12
9821	Pyrazole Compounds : Synthesis, molecular structure, chemical reactivity, experimental and theoretical DFT FTIR spectra. <i>Materials Today: Proceedings</i> , 2019, 13, 956-963.	0.9	7
9822	Maltol- and Allomaltol-Derived Oxidopyrylium Ylides: Methyl Substitution Pattern Kinetically Influences [5 + 3] Dimerization versus [5 + 2] Cycloaddition Reactions. <i>Journal of Organic Chemistry</i> , 2019, 84, 14670-14678.	1.7	4
9823	Double-Hybrid Functionals and Tailored Basis Set: Fullerene (C ₆₀) Dimer and Isomers as Test Cases. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10040-10046.	1.1	11

#	ARTICLE	IF	CITATIONS
9824	Mechanism of the Iron(0)-Catalyzed Hydrosilylation of Aldehydes: A Combined DFT and Experimental Investigation. <i>Organometallics</i> , 2019, 38, 4105-4114.	1.1	13
9825	Electronic structures and optical properties of CuMgVO ₄ and AgMgVO ₄ : a first-principles study. <i>Journal of the Ceramic Society of Japan</i> , 2019, 127, 50-55.	0.5	1
9826	Plasmon-Induced Dimerization of Thiazolidine-2,4-dione on Silver Nanoparticles: Revealed by Surface-Enhanced Raman Scattering Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9770-9780.	1.1	10
9827	Approximating Periodic Potential Energy Surfaces with Sparse Trigonometric Interpolation. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9677-9684.	1.2	3
9828	Spectroscopic and Computational Evidence of Intramolecular Au ^I ...H ⁺ Hydrogen Bonding. <i>Angewandte Chemie</i> , 2019, 131, 2033-2038.	1.6	19
9829	Synthesis, crystal structures and electrochemical properties of ferrocenyl imidazole derivatives. <i>Heliyon</i> , 2019, 5, e02580.	1.4	4
9830	Templating metastable Pd ₂ carboxylate aggregates. <i>Chemical Science</i> , 2019, 10, 1823-1830.	3.7	15
9831	Retrofitting metal-organic frameworks. <i>Nature Communications</i> , 2019, 10, 4921.	5.8	30
9832	Restoring the iso-orbital limit of the kinetic energy density in relativistic density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 174114.	1.2	7
9833	How do halogen atoms affect Xe-Mo double bond? A theoretical study of X ₂ XeMoY ₂ (X = F, Cl, Br; Y = F, Cl, Br). <i>Journal of Chemical Physics</i> , 2019, 151, 174114.	1.1	1
9834	Modeling molecularly imprinted polymer mechanics. <i>Journal of Applied Polymer Science</i> , 2019, 141, 51-75.		3
9835	Computationally Assisted Mechanistic Investigation into Hypervalent Iodine Catalysis: Cyclization of <i>N</i> -Allylbenzamide. <i>Journal of Organic Chemistry</i> , 2019, 84, 15605-15613.	1.7	13
9836	A combined experimental and quantum chemical studies on the structure and binding preferences of picolinamide based ligands with uranyl nitrate. <i>Polyhedron</i> , 2019, 171, 486-492.	1.0	2
9837	<i>N</i> -Ethyl Carbazole Derived β -Cyanamide Based Fluorophores: Consolidated Spectroscopic, Viscosity and DFT Studies. <i>ChemistrySelect</i> , 2019, 4, 11966-11978.	0.7	3
9838	A computational study of the electronic structure and optical properties of the complex TeO ₂ /TeO ₃ oxides as advanced materials for nonlinear optics. <i>Materials Research Express</i> , 2019, 6, 125903.	0.8	2
9839	Emission solvatochromic, solid-state and aggregation-induced emissive β -pyrones and emission-tuneable 1H-pyridines by Michael addition-cyclocondensation sequences. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 2684-2703.	1.3	4
9840	Investigation of the reactivity indices for the formation of substituted dinitroanilines and correlations to their dockings on β -tubulin of <i>Plasmodium falciparum</i> . <i>Journal of Molecular Modeling</i> , 2019, 25, 342.	0.8	1
9841	Resonant X-ray Sum-Frequency-Generation Spectroscopy of K-Edges in Acetyl Fluoride. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6832-6839.	2.3	5

#	ARTICLE	IF	CITATIONS
9842	Radiolytic Oxidation of Two Inverse Dipeptides, Methionineâ€“Valine and Valineâ€“Methionine: A Joint Experimental and Computational Study. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9087-9097.	1.2	4
9843	Unimolecular Exciplexes by Ugi Four-Component Reaction. <i>Frontiers in Chemistry</i> , 2019, 7, 717.	1.8	2
9844	Fragmentation Spectra Prediction and DNA Adducts Structural Determination. <i>Journal of the American Society for Mass Spectrometry</i> , 2019, 30, 2771-2784.	1.2	10
9845	Many-body corrected tight-binding Hamiltonians for an accurate quasiparticle description of topological insulators of the Bi_2Se_3 family. <i>Physical Review B</i> , 2019, 100, .	1.1	17
9846	Complexities of the Reaction Mechanisms of CC Double Bond Reduction in Mammalian Fatty Acid Synthase Studied with Quantum Mechanics/Molecular Mechanics Calculations. <i>ACS Catalysis</i> , 2019, 9, 11404-11412.	5.5	9
9847	Studies of Halogen Bonding Induced by Pentafluorosulfanyl Aryl Iodides: A Potential Group of Halogen Bond Donors in a Rational Drug Design. <i>Molecules</i> , 2019, 24, 3610.	1.7	11
9848	Twisting the TAPPs: Bay-Substituted Non-Planar Tetraazaperyrenes and their Reduced Anions. <i>Chemistry - A European Journal</i> , 2019, 25, 14669-14678.	1.7	12
9849	Rhodium Complexes in P-H Bond Activation Reactions. <i>Chemistry - A European Journal</i> , 2019, 25, 15915-15928.	1.7	13
9850	Early Main Group Metal Catalysts for Imine Hydrosilylation. <i>Chemistry - A European Journal</i> , 2019, 25, 16141-16147.	1.7	23
9851	Performance of Density Functional Theory for Transition Metal Oxygen Bonds. <i>ChemPhysChem</i> , 2019, 20, 3210-3220.	1.0	9
9852	CpRu Complexes Containing Water Soluble Phosphane PTA and Natural Purines Adenine, Guanine and Theophylline: Synthesis, Characterization, and Antiproliferative Properties. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 4078-4086.	1.0	11
9853	Identification of molecular vibrations associated with tacticity in polypropylene: Density functional theory-based simulations. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2019, 57, 1378-1385.	2.4	1
9854	Theoretical Investigation of Optical and Nonlinear Optical (NLO) Properties of 3-Azabenzanthrone Analogues : DFT and TD-DFT Approach.. <i>ChemistrySelect</i> , 2019, 4, 10033-10045.	0.7	21
9855	Pyrene Based NLOphoric Diethyl Coumarin-Chalcone and Their Red Emitting OBO Difluoride Complex: Synthesis, Solvatochromism, Z-scan, and Detailed TD-DFT Studies. <i>ChemistrySelect</i> , 2019, 4, 10385-10400.	0.7	10
9856	High-Performance Inverted Planar Perovskite Solar Cells Enhanced by Thickness Tuning of New Dopant-Free Hole Transporting Layer. <i>Small</i> , 2019, 15, e1904715.	5.2	47
9857	Oxidation of Isoprene by Neutral Iron Oxide Nanoclusters in the Gas Phase. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25949-25956.	1.5	8
9858	Photochemistry of (η^3 -allyl)Ru(CO) ₃ X Precursors for Photoassisted Chemical Vapor Deposition. <i>Organometallics</i> , 2019, 38, 4363-4370.	1.1	4
9859	Simple exchange hole models for long-range-corrected density functionals. <i>Journal of Chemical Physics</i> , 2019, 151, 094106.	1.2	5

#	ARTICLE	IF	CITATIONS
9860	Theoretical Study of Ternary CoSP Semiconductor: A Candidate for Photovoltaic Applications. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900111.	1.3	1
9861	Electronic properties of novel bismuthene nanosheets with adsorption studies of G-series nerve agent molecules – a DFT outlook. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 125975.	0.9	21
9862	New hexanuclear FeIII clusters with the gem-diol hydrated form of di(2-pyridyl)ketone and carboxylato ligands: Crystal structures and magnetic properties. <i>Polyhedron</i> , 2019, 174, 114165.	1.0	3
9863	Consecutive Marcus Electron and Proton Transfer in Heme Peroxidase Compound II-Catalysed Oxidation Revealed by Arrhenius Plots. <i>Scientific Reports</i> , 2019, 9, 14092.	1.6	3
9864	Developing a self-consistent AGB wind model – II. Non-classical, non-equilibrium polymer nucleation in a chemical mixture. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 489, 4890-4911.	1.6	26
9865	Unconventional phase III of high-pressure solid hydrogen. <i>Physical Review B</i> , 2019, 100, .	1.1	10
9866	The Laboratory Millimeter and Submillimeter Rotational Spectrum of Lactaldehyde and an Astronomical Search in Sgr B2(N), Orion-KL, and NGC 6334I. <i>Astrophysical Journal</i> , 2019, 883, 18.	1.6	8
9867	Towards deep-blue phosphorescence: molecular design and property prediction of iridium complexes with pyridinylphosphinate ancillary ligand. <i>Applied Organometallic Chemistry</i> , 2019, 33, e5167.	1.7	5
9868	Kinetic, Spectroscopic, and DFT Studies of Novel Oxidation of Acetylsalicylic Acid by NaIO ₄ Using Micro-amount of Os(VIII) As a Homogeneous Catalyst in Alkaline Medium. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 2023-2031.	0.1	3
9869	Binary Donor–Acceptor Adducts of Tetrathiafulvalene Donors with Cyclic Trimetallic Monovalent Coinage Metal Acceptors. <i>Inorganic Chemistry</i> , 2019, 58, 15303-15319.	1.9	9
9870	Application of quantum chemical methods in polymer chemistry. <i>International Reviews in Physical Chemistry</i> , 2019, 38, 343-403.	0.9	22
9871	Electronic structure from equivalent differential equations of Hartree–Fock equations. <i>Chinese Physics B</i> , 2019, 28, 087101.	0.7	7
9872	The synthesis and spectroscopic characterization of (+)-demethoxyaspidospermine: Density functional theory calculations of the structural, electronic, and non-linear optic and spectroscopic properties. <i>Journal of Chemical Research</i> , 2019, 43, 531-541.	0.6	7
9873	Ex Vivo Analysis of Tryptophan Metabolism Using ¹⁹ F NMR. <i>ACS Chemical Biology</i> , 2019, 14, 1866-1873.	1.6	5
9874	Performance Analysis and Optimization of Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) for Vertical Excitation Energies and Singlet–Triplet Energy Gaps. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7991-8000.	1.1	27
9875	Molecular Dynamics Study on the Mechanism of Graphene Oxide to Destabilize Oil/Water Emulsion. <i>Journal of Physical Chemistry C</i> , 2019, 123, 22989-22999.	1.5	34
9876	Structural, mechanical, and electronic properties of 25 kinds of III–V binary monolayers: A computational study with first-principles calculation*. <i>Chinese Physics B</i> , 2019, 28, 086105.	0.7	29
9877	A DFT mechanistic and kinetic study on the reaction of phloroglucinol with [•] OH in different media: Hydrogen atom transfer versus oxidation. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950017.	1.8	6

#	ARTICLE	IF	CITATIONS
9878	Computational Investigation into the Ni(SeNHC2(CN)2)2 and Ni(SNHC2(CN)2)2 Complexes as Potential Catalysts for Hydrogen Production. Journal of Physical Chemistry A, 2019, 123, 7822-7827.	1.1	2
9879	A DFT mechanistic, thermodynamic and kinetic study on the reaction of 1, 3, 5-trihydroxybenzene and 2, 4, 6-trihydroxyacetophenone with H_2O_2 in different media. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950023.	1.8	5
9880	Multiscale Computational Study on the Catalytic Mechanism of the Nonmetallo Amidase Maleamate Amidohydrolase (NicF). Journal of Physical Chemistry A, 2019, 123, 7710-7719.	1.1	1
9881	Theoretical study for chromen azodyes derivative compounds as anti-corrosive. Journal of Physics: Conference Series, 2019, 1234, 012054.	0.3	0
9882	Switchable second-order nonlinear optical response of platinum-sensitized dithienylethenes. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950022.	1.8	0
9883	ESIPT-rhodol derivatives with enhanced Stokes shift: Synthesis, photophysical properties, viscosity sensitivity and DFT studies. Journal of Molecular Liquids, 2019, 294, 111626.	2.3	13
9884	Effects of Core Modification on Electronic Properties of <i>para</i> -Benziporphyrins. Inorganic Chemistry, 2019, 58, 12069-12082.	1.9	20
9885	DFT and QSAR Studies of Ethylene Polymerization by Zirconocene Catalysts. ACS Catalysis, 2019, 9, 9339-9349.	5.5	25
9886	Bowl-shaped fluorescent liquid crystals derived from 4- <i>tert</i> -butyl calix[4]arene and <i>trans</i> -cinnamic acid derivatives. New Journal of Chemistry, 2019, 43, 15575-15584.	1.4	9
9887	Theoretical study of the photoconduction and photomagnetism of the BPY[Ni(dmit)2]2 molecular crystal. Dalton Transactions, 2019, 48, 13789-13798.	1.6	1
9888	Machine learning prediction of accurate atomization energies of organic molecules from low-fidelity quantum chemical calculations. MRS Communications, 2019, 9, 891-899.	0.8	38
9889	DFT/MRCI-R2018 study of the photophysics of the zinc(<i>scpi</i>) tripyrindione radical: non-Kasha emission?. Physical Chemistry Chemical Physics, 2019, 21, 19857-19867.	1.3	10
9890	Synthesis, characterizations and single crystal structure of di-nuclear azido-bridged Cd(II) coordination polymer with Schiff base precursor (H2LpentOMe): DFT, fluorescence, solvatochromism and in vitro antimicrobial assay. Inorganica Chimica Acta, 2019, 496, 119069.	1.2	16
9891	Spectroscopic (FT-IR, NMR) and Computational Investigation of 2-(2-Aminoethyl)-1,2,3,4,9-Tetrahydrocarbazole: NBO, NLO, FMO, MEP Analysis. Journal of Structural Chemistry, 2019, 60, 1267-1284.	0.3	12
9892	Structural evolution and electronic properties of Au2Gen ⁻ /O (n=1~8) clusters: Anion photoelectron spectroscopy and theoretical calculations. Chinese Journal of Chemical Physics, 2019, 32, 229-240.	0.6	9
9893	<i>Ab initio</i> simulations of x-ray emission spectroscopy with the mml:math $\text{xmlns:mml}="http://www.w3.org/1998/Math/MathML">\text{mml:mrow}<\text{mml:mi}>G<\text{mml:mi}>\text{mml:mi}>W<\text{mml:mi}>\text{mml:mo}>8<\text{mml:mo}>$ Bethe-Salpeter equation method. Physical Review B, 2019, 100, .		
9894	Yellow-red emitting, methoxy substituted triphenylamine-based styryl derivatives: Synthesis, photophysical properties, viscosity sensitivity, aggregation induced emission, NLO properties, and DFT study. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 384, 112027.	2.0	7
9895	Concentration dependent energy levels shifts in donor-acceptor mixtures due to intermolecular electrostatic interaction. Scientific Reports, 2019, 9, 12424.	1.6	8

#	ARTICLE	IF	CITATIONS
9896	A trade-off for covalent and intercalation binding modes: a case study for Copper (II) ions and singly modified DNA nucleoside. <i>Scientific Reports</i> , 2019, 9, 12602.	1.6	2
9897	Accelerated computation of free energy profile at <i>ab initio</i> quantum mechanical/molecular mechanical accuracy <i>via</i> a semi-empirical reference potential. II. Recalibrating semi-empirical parameters with force matching. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20595-20605.	1.3	30
9898	Two-dimensional Na _x SiS as a promising anode material for rechargeable sodium-based batteries: <i>ab initio</i> material design. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24326-24332.	1.3	13
9899	Tuning receptors for the encapsulation of beryllium ²⁺ . <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19660-19666.	1.3	8
9900	Theoretical studies on the energy structures and optical properties of copper cysteamine – a novel sensitizer. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21084-21093.	1.3	7
9901	Modeling of silicon- and aluminum-doped phosphorene nanoflakes. <i>Journal of Molecular Modeling</i> , 2019, 25, 292.	0.8	4
9902	Solvent dependent ESI-collisionally induced dissociation of protonated nitenpyram. <i>International Journal of Mass Spectrometry</i> , 2019, 445, 116207.	0.7	3
9903	AIRBED: A Simplified Density Functional Theory Model for Physisorption on Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5628-5634.	2.3	8
9904	Emission Energies and Stokes Shifts for Single Polycyclic Aromatic Hydrocarbon Sheets in Comparison to the Effect of Excimer Formation. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5592-5597.	2.1	18
9905	Charge-transfer electronic states in organic solar cells. <i>Nature Reviews Materials</i> , 2019, 4, 689-707.	23.3	229
9906	Coupled alkali halide color centers: Fractional charge errors, fractional spin errors, and a failure of spin symmetry breaking produce challenging tests for condensed-phase electronic structure calculations. <i>Journal of Chemical Physics</i> , 2019, 151, 064109.	1.2	0
9907	The photophysical properties and electronic structures of bis[1]benzothieno[6,7- <i>d</i> :6,7- <i>d'</i>]benzo[1,2- <i>b</i> :4,5- <i>b'</i>]dithiophene (BBTBDT) derivatives as hole-transporting materials for organic light-emitting diodes (OLEDs). <i>New Journal of Chemistry</i> , 2019, 43, 15899-15909.	1.4	17
9908	Adsorption Behavior of CH ₄ Gas Molecule on the MoX ₂ (S, Se, Te) Monolayer: The DFT Study. <i>Nanoscale Research Letters</i> , 2019, 14, 293.	3.1	15
9909	Probing the Partial Activation of Water by Open-Shell Interactions, Cl(H ₂ O) ₄ . <i>Journal of Physical Chemistry A</i> , 2019, 123, 8657-8673.	1.1	9
9910	Geometries and NMR properties of cisplatin and transplatin revisited at the four-component relativistic level. <i>Mendeleev Communications</i> , 2019, 29, 315-317.	0.6	9
9911	Hydroxyl radical-mediated degradation of salicylic acid and methyl paraben: an experimental and computational approach to assess the reaction mechanisms. <i>Environmental Science and Pollution Research</i> , 2019, 26, 33125-33134.	2.7	10
9912	Chiral Phosphoric Acid-Catalyzed Enantioselective Direct Arylation of Iminoquinones: A Case Study of the Model Selectivity. <i>Journal of Organic Chemistry</i> , 2019, 84, 13473-13482.	1.7	7
9913	Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5601-5613.	2.3	32

#	ARTICLE	IF	CITATIONS
9914	Photoelectron Spectroscopy of Molecules Beyond the Electric Dipole Approximation. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5483-5494.	2.3	5
9915	Hierarchy of Commonly Used DFT Methods for Predicting the Thermochemistry of Rh-Mediated Chemical Transformations. <i>ACS Omega</i> , 2019, 4, 15435-15443.	1.6	11
9916	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21094-21103.	1.3	47
9917	Correlation between molecular charge densities and sensitivity of nitrogen-rich heterocyclic nitroazole derivative explosives. <i>Journal of Molecular Modeling</i> , 2019, 25, 314.	0.8	18
9918	Azido bridged binuclear copper(II) Schiff base compound: synthesis, structure and electrical properties. <i>New Journal of Chemistry</i> , 2019, 43, 16255-16263.	1.4	9
9919	Reactivity of HCO with CH ₃ and NH ₂ on Water Ice Surfaces. A Comprehensive Accurate Quantum Chemistry Study. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 2158-2170.	1.2	55
9920	Dielectric relaxation studies of aqueous l-glutamine-ethanol mixtures in the microwave frequency range. <i>Journal of Molecular Liquids</i> , 2019, 293, 111506.	2.3	5
9921	LCOFs: Role of the excited state hydrogen bonding in the detection for nitro-explosives. <i>Journal of Luminescence</i> , 2019, 215, 116733.	1.5	7
9922	Group-transfer chemistry at transition metal centers in bulky alkoxide ligand environments. <i>Coordination Chemistry Reviews</i> , 2019, 400, 213044.	9.5	12
9923	Analytic first-order derivatives of partially contracted <i>n</i> -electron valence state second-order perturbation theory (PC-NEVPT2). <i>Journal of Chemical Physics</i> , 2019, 151, 114103.	1.2	19
9924	Theoretical study of H-atom abstraction reactions from CH ₃ CH ₂ OCH ₂ CH ₃ , CHF ₂ CF ₂ OCH ₂ CF ₃ and CF ₃ CH ₂ OCH ₃ by NO ₃ radical & subsequent degradation. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 93, 107453.	1.3	6
9925	Kinetics and mechanism of the $\text{CH}_3 + \text{CH}_3$ reaction with H^+ . <i>Chemical Physics Letters</i> , 2019, 734, 136699.	1.2	1
9926	3-(p-nitrophenyl)Coumarin derivatives: Synthesis, linear and nonlinear optical properties. <i>Optical Materials</i> , 2019, 96, 109328.	1.7	19
9927	Eu(III) and Tb(III) complexes of 6-fold coordinating ligands showing high affinity for the hydrogen carbonate ion: a spectroscopic and thermodynamic study. <i>Dalton Transactions</i> , 2019, 48, 1202-1216.	1.6	20
9928	Designing air-stable cyclometalated Fe(II) complexes: stabilization via electrostatic effects. <i>Dalton Transactions</i> , 2019, 48, 374-378.	1.6	12
9929	Ion reactions in atmospherically-relevant clusters: mechanisms, dynamics and spectroscopic signatures. <i>Faraday Discussions</i> , 2019, 217, 342-360.	1.6	3
9930	Ambipolar Discotic Liquid Crystals Built Around Platinum Diimine-Dithiolene Cores. <i>Chemistry - A European Journal</i> , 2019, 25, 5719-5732.	1.7	9
9931	Synthesis, Characterization and Theoretical Calculation of New Azo Dyes Derived from [1,5a]Pyrimidine Having Solvatochromic Properties. <i>Journal of Heterocyclic Chemistry</i> , 2019, 56, 1101-1110.	1.4	5

#	ARTICLE	IF	CITATIONS
9932	The electron affinities of TCNE and TCNQ: the effect of silicon substitution. <i>Structural Chemistry</i> , 2019, 30, 289-301.	1.0	2
9933	Valence bonds in planar and quasi-planar boron disks. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 729-735.	1.3	5
9934	Constructing organic superacids from superhalogens is a rational route as verified by DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2804-2815.	1.3	15
9935	Investigation of cation binding and sensing by new crown ether core substituted naphthalene diimide systems. <i>New Journal of Chemistry</i> , 2019, 43, 2011-2018.	1.4	11
9936	Two-dimensional electronic-vibrational spectroscopic study of conical intersection dynamics: an experimental and electronic structure study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14153-14163.	1.3	32
9937	Extremely large differences in DFT energies for nitrogenase models. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2480-2488.	1.3	56
9938	Pushing the limits of concertedness. A waltz of wandering carbocations. <i>Chemical Science</i> , 2019, 10, 2159-2170.	3.7	21
9939	Theoretical Study of the Charge Transfer Exciton Binding Energy in Semiconductor Materials for Polymer:Fullerene-Based Bulk Heterojunction Solar Cells. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1233-1242.	1.1	12
9940	Insight into the optical properties of meso-pentafluorophenyl(PFP)-BODIPY: An attractive platform for functionalization of BODIPY dyes. <i>Computational and Theoretical Chemistry</i> , 2019, 1150, 110-120.	1.1	3
9941	A first step towards quantum energy potentials of electron pairs. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4215-4223.	1.3	11
9942	Does the Neophyl-like Rearrangement Play a Decisive Role in Intramolecular Cyclization of Iminyl Radicals? A Combined Quantum Chemistry and Numerical Simulation Investigation of the Cyclization Mechanism and Product Distributions of Bicyclic 2-Allyl-2-methyl-2,3-dihydro-1 <i>H</i> -inden-1-iminyl Radical and Several Iminyl Model Compounds. <i>Journal of Organic Chemistry</i> , 2019, 84, 2721-2731.	1.7	4
9943	Diphosphazane-monoxide and Phosphine-sulfonate Palladium Catalyzed Ethylene Copolymerization with Polar Monomers: A Computational Study. <i>Organometallics</i> , 2019, 38, 638-646.	1.1	25
9944	NLO-phoric Triphenylamine Derived Donor-Acceptor Donor Based Colorants: Synthesis, Spectroscopic, Density Functional Theory and ϵ -scan Studies. <i>Photochemistry and Photobiology</i> , 2019, 95, 931-945.	1.3	11
9945	Reduced-Scaling Approach for Configuration Interaction Singles and Time-Dependent Density Functional Theory Calculations Using Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1690-1704.	2.3	10
9946	Sub-Band Gap Absorption Mechanisms Involving Oxygen Vacancies in Hydroxyapatite. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4856-4865.	1.5	26
9947	Density Functional Theory Calculations of Structural, Electronic, and Magnetic Properties of the 3d Metal Trifluorides MF ₃ (M = Ti-Ni) in the Solid State. <i>Journal of Computational Chemistry</i> , 2019, 40, 1190-1197.	1.5	14
9948	Role of Mineral Surfaces in Prebiotic Chemical Evolution. In <i>Silico Quantum Mechanical Studies</i> . <i>Life</i> , 2019, 9, 10.	1.1	44
9949	XPS and DFT investigations of corrosion inhibition of substituted benzylidene Schiff bases on mild steel in hydrochloric acid. <i>Applied Surface Science</i> , 2019, 476, 861-877.	3.1	162

#	ARTICLE	IF	CITATIONS
9950	Complexation of luteolin with lead (II): Spectroscopy characterization and theoretical researches. Journal of Inorganic Biochemistry, 2019, 193, 25-30.	1.5	19
9951	Noncovalent Porphyrin@Graphene Oxide Nanohybrids: The pH-Dependent Behavior. Journal of Physical Chemistry C, 2019, 123, 3368-3380.	1.5	25
9952	Electronic Structure and Band Alignments of Various Phases of Titania Using the Self-Consistent Hybrid Density Functional and DFT+U Methods. Frontiers in Chemistry, 2019, 7, 47.	1.8	12
9953	Novel D-π-A organic dyes for DSSCs based on dibenzo[b,h][1,6]naphthyridine as a π-bridge. Dyes and Pigments, 2019, 164, 188-197.	2.0	27
9954	Introducing Asymmetry Induced by Benzene Substitution in a Rigid Fused π Spacer of DπA-Type Solar Cells: A Computational Investigation. Journal of Physical Chemistry C, 2019, 123, 4007-4021.	1.5	41
9955	A computational study on ligand assisted <i>vs.</i> ligand participation mechanisms for CO ₂ hydrogenation: importance of bifunctional ligand based catalysts. Physical Chemistry Chemical Physics, 2019, 21, 3932-3941.	1.3	16
9956	Instanton rate constant calculations using interpolated potential energy surfaces in nonredundant, rotationally and translationally invariant coordinates. Journal of Computational Chemistry, 2019, 40, 866-874.	1.5	10
9957	The plutonium chemistry of Pu+O ₂ system: the theoretical investigation of the plutonium-oxygen interaction. Journal of the Iranian Chemical Society, 2019, 16, 1157-1162.	1.2	4
9958	Revised M11 Exchange-Correlation Functional for Electronic Excitation Energies and Ground-State Properties. Journal of Physical Chemistry A, 2019, 123, 2966-2990.	1.1	76
9959	Atomic photoionization cross sections beyond the electric dipole approximation. Journal of Chemical Physics, 2019, 150, 044306.	1.2	5
9960	3D meso-nanostructures in cleaved and nanolithographed Mg-Al-hydroxysilicate (clinochlore): Topology, crystal-chemistry, and surface properties. Applied Clay Science, 2019, 169, 74-80.	2.6	11
9961	Dioxygen Reduction to Hydrogen Peroxide by a Molecular Mn Complex: Mechanistic Divergence between Homogeneous and Heterogeneous Reductants. Journal of the American Chemical Society, 2019, 141, 4379-4387.	6.6	51
9962	The Interaction of Water with <i>cis</i> and <i>trans</i> {Ru(bpy) ₂ (PTA) ₂ } ²⁺ (PTA = 1,3,5-Triaza-7-phosphadamantane) Studied by Neutron Scattering and Ab Initio Calculations. European Journal of Inorganic Chemistry, 2019, 2019, 1162-1169.	1.0	8
9963	Influence of acceptors in NLOphoric acenaphthene and morpholine-thiourea hybrid dyes: Photophysical, viscosity, DFT and Z-Scan study. Optical Materials, 2019, 89, 178-190.	1.7	7
9964	A General Model to Explain the Isoselectivity of Olefin Polymerization Catalysts. , 2019, , 269-285.		3
9965	Hybrid Functional Study of the Electro-oxidation of Water on Pristine and Defective Hematite (0001). Journal of Physical Chemistry C, 2019, 123, 2820-2827.	1.5	12
9966	Extending the π-electron conjugation in 2D planar graphitic carbon nitride: efficient charge separation for overall water splitting. Journal of Materials Chemistry A, 2019, 7, 3757-3771.	5.2	128
9967	Unveiling anharmonic coupling by means of excited state <i>ab initio</i> dynamics: application to diarylethene photoreactivity. Physical Chemistry Chemical Physics, 2019, 21, 3606-3614.	1.3	28

#	ARTICLE	IF	CITATIONS
9968	Theoretical studies on photo-induced cycloaddition and (6-4) reactions of the thymidine:4-thiothymidine dimer in a DNA duplex. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2006-2016.	1.3	8
9969	A first-principles study of the electronic, structural, and optical properties of CrN and Mo:CrN clusters. <i>Ceramics International</i> , 2019, 45, 17094-17102.	2.3	4
9970	Reassessment of the Mechanisms of Thermal C-H Bond Activation of Methane by Cationic Magnesium Oxides: A Critical Evaluation of the Suitability of Different Density Functionals. <i>ChemPhysChem</i> , 2019, 20, 1812-1821.	1.0	5
9971	Ultrasound induced green synthesis of pyrazolo-pyridines as novel corrosion inhibitors useful for industrial pickling process: Experimental and theoretical approach. <i>Results in Physics</i> , 2019, 13, 102344.	2.0	28
9972	Fast hybrid density-functional computations using plane-wave basis sets. <i>Electronic Structure</i> , 2019, 1, 015009.	1.0	29
9973	A high-spin ground-state donor-acceptor conjugated polymer. <i>Science Advances</i> , 2019, 5, eaav2336.	4.7	72
9974	Triphenylamine and N-phenyl carbazole-based coumarin derivatives: Synthesis, solvatochromism, acidochromism, linear and nonlinear optical properties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 382, 111937.	2.0	43
9975	Relaxation dynamics of L-alanine in water medium investigated by dielectric relaxation spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 222, 117274.	2.0	3
9976	A DFT Investigation on the Structure, Spectroscopy (FTIR and NMR), Donor-Acceptor Interactions and Non-Linear Optic Properties of (1,2-D)Dehydroaspidospermidine. <i>ChemistrySelect</i> , 2019, 4, 6870-6878.	0.7	14
9977	A Simplified Spin-Flip Time-Dependent Density Functional Theory Approach for the Electronic Excitation Spectra of Very Large Diradicals. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5815-5825.	1.1	17
9978	Mechanism of the Palladium-Catalyzed C(sp ³)-H Arylation of Aliphatic Amines: Unraveling the Crucial Role of Silver(I) Additives. <i>ACS Catalysis</i> , 2019, 9, 6672-6680.	5.5	38
9979	Multicenter Bonding and the Electron Deficient Molecules with Special Emphasis to Boron and Aluminium Compounds. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 1116-1121.	0.1	2
9980	Elucidating the Doping Effect on the Electronic Structure of Thiolate-Protected Silver Superatoms by Photoelectron Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 11637-11641.	7.2	41
9981	A comprehensive study on electronic structure and optical properties of carbon nanotubes with doped B, Al, Ga, Si, Ge, N, P and As and different diameters. <i>Journal of Alloys and Compounds</i> , 2019, 802, 25-35.	2.8	30
9982	Triplet and Singlet (n,π*) Excited States of 4-H-Pyran-4-one Characterized by Cavity Ringdown Spectroscopy and Quantum-Chemical Calculations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6269-6280.	1.1	5
9983	Benchmark of Density Functionals for the Calculation of the Redox Potential of Fe ³⁺ /Fe ²⁺ Within Protein Coordination Shells. <i>Frontiers in Chemistry</i> , 2019, 7, 391.	1.8	14
9984	Valence-Shell Electron-Pair Repulsion Theory Revisited: An Explanation for Core Polarization. <i>Chemistry - A European Journal</i> , 2019, 25, 10938-10945.	1.7	7
9985	Design and Synthesis of an Activatable Photoacoustic Probe for Hypochlorous Acid. <i>Analytical Chemistry</i> , 2019, 91, 9086-9092.	3.2	37

#	ARTICLE	IF	CITATIONS
9986	Rational Molecular Design of Dibenzo[<i>a,c</i>]phenazine-Based Thermally Activated Delayed Fluorescence Emitters for Orange-Red OLEDs with EQE up to 22.0%. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 26144-26151.	4.0	73
9987	Modeling L2,3-edge X-ray absorption spectroscopy with linear response exact two-component relativistic time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2019, 150, 234103.	1.2	28
9988	Antioxidative activity analyses of some pyridazine derivatives using computational methods. <i>Chemical Papers</i> , 2019, 73, 3105-3113.	1.0	1
9989	Decreasing Exciton Binding Energy in Two-Dimensional Halide Perovskites by Lead Vacancies. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3820-3827.	2.1	27
9990	Tuning the supramolecular chirality and optoelectronic performance of chiral perylene diimide nanowires <i>via N</i> -substituted side chain engineering. <i>Journal of Materials Chemistry C</i> , 2019, 7, 8688-8697.	2.7	23
9991	A theoretical investigation into the first-row transition metal ²⁺ adducts. <i>Inorganic Chemistry Frontiers</i> , 2019, 6, 2071-2081.	3.0	12
9992	Tracking pereirole and flavopereirole in pau-pereira using Raman and SERS spectroscopies. <i>New Journal of Chemistry</i> , 2019, 43, 11200-11208.	1.4	2
9993	Molecular modeling and computational study of the chiral-dependent structures and properties of self-assembling diphenylalanine peptide nanotubes. <i>Journal of Molecular Modeling</i> , 2019, 25, 199.	0.8	27
9994	Theoretical investigation on the interaction of benzazaborole derivatives with iodide ion: Structural, binding and fluorescence properties analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 92, 32-43.	1.3	3
9995	Uncovering the Binding Mode of \hat{I}^3 -Secretase Inhibitors. <i>ACS Chemical Neuroscience</i> , 2019, 10, 3398-3403.	1.7	21
9996	Analysis of the Puzzling Exchange-Coupling Constants in a Series of Heterobimetallic Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 9150-9160.	1.9	2
9997	Accurate quantum chemical energies for 133,000 organic molecules. <i>Chemical Science</i> , 2019, 10, 7449-7455.	3.7	53
9998	Efficient simulation of overtones and combination bands in resonant Raman spectra. <i>Journal of Chemical Physics</i> , 2019, 150, 214102.	1.2	25
9999	A computational study on the redox properties and binding affinities of iron complexes of hydroxypyridinones. <i>Journal of Molecular Modeling</i> , 2019, 25, 172.	0.8	4
10000	Heteroatom Bay-Annulated Perylene Bisimides: New Materials for Organic Field Effect Transistors. <i>ACS Applied Electronic Materials</i> , 2019, 1, 1378-1386.	2.0	31
10001	Theoretical study on the mechanism and chemoselectivity in gold(⁺)-catalyzed cycloisomerization of \hat{I}^2, \hat{I}^2 -disubstituted <i>ortho</i> -(alkynyl)styrenes. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2701-2712.	2.3	13
10002	Mechanistic investigation-inspired activation mode of DBU and the function of the \hat{I}^2 -diazo group in the reaction of the \hat{I}^2 -amino ketone compound and EDA: [DBU-H] ⁺ -DMF-H ₂ O and \hat{I}^2 -diazo as strong N-terminal nucleophiles. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2678-2686.	2.3	2
10003	Ab initio kinetics for pyrolysis and combustion systems. <i>Computer Aided Chemical Engineering</i> , 2019, , 115-167.	0.3	27

#	ARTICLE	IF	CITATIONS
10004	Push-pull isomers of indolizino[6,5,4,3- <i>def</i>]phenanthridine decorated with a triarylboron moiety. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 6470-6477.	1.5	3
10005	Computational Multinuclear NMR of Platinum Complexes: A Relativistic Four-Component Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4908-4920.	1.1	14
10006	Benchmarks for Electronically Excited States with CASSCF Methods. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4170-4179.	2.3	19
10007	Combined Experimental and Theoretical Studies on the Radical Nucleophile Addition Reaction for Sulfide- and Selenide-Centered Anions. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5035-5042.	1.1	0
10008	Spectroscopic diagnostic for the ring-size of carbohydrates in the gas phase: furanose and pyranose forms of GalNAc. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12460-12467.	1.3	13
10009	Range-separated hybrid density functionals made simple. <i>Journal of Chemical Physics</i> , 2019, 150, 201102.	1.2	60
10010	Combined use of tandem mass spectrometry and computational chemistry to study 2- <i>H</i> -chromenes from <i>Piper aduncum</i> . <i>Journal of Mass Spectrometry</i> , 2019, 54, 634-642.	0.7	3
10011	Prediction of aqueous solubility by treatment of COSMO-RS data with empirical solubility equations: the roles of global orbital cut-off and COSMO solvent radius. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	9
10012	Structures of [GPGG ⁺ H ⁺ H ₂ O] ⁺ and [GPGG ⁺ H ⁺ H ₂ O ⁺ NH ₂ CH ₂] ⁺ ions; evidence of rearrangement prior to dissociation. <i>International Journal of Mass Spectrometry</i> , 2019, 442, 51-57.	0.7	0
10013	Ionized, electron-attached, and excited states of molecular systems with spin-orbit coupling: Two-component <i>GW</i> and Bethe-Salpeter implementations. <i>Journal of Chemical Physics</i> , 2019, 150, 204116.	1.2	48
10014	Graphene Nanobelts, Möbius and Higher Order Möbius Strips Formed from Graphene. A Combined CASSCF/DFT Study. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 723-729.	0.1	0
10015	Push-Pull Chromophores Based on the Naphthalene Scaffold: Potential Candidates for Optoelectronic Applications. <i>Materials</i> , 2019, 12, 1342.	1.3	29
10016	Connecting Solution-Phase to Single-Molecule Properties of Ni(Salophen). <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3525-3530.	2.1	8
10017	New dyads based on trifluoromethylated phthalocyanine derivatives and substituted fullerene with possible application photoinduced electron transfer. <i>Journal of Fluorine Chemistry</i> , 2019, 224, 113-120.	0.9	15
10018	Kinetic Investigations of the CH(X ²) Radical Reaction with Cyclopentadiene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5692-5703.	1.1	7
10019	Optical Spectra and Fluorescence Quenching in Azaacenes Bearing Five-Membered Rings. <i>ChemPhotoChem</i> , 2019, 3, 755-762.	1.5	6
10020	Insights into the halochromism of a bithiophene π^* probe. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 222, 117264.	2.0	2
10021	Theoretical Search for the Highest Valence States of the Coinage Metals: Roentgenium Heptafluoride May Exist. <i>Inorganic Chemistry</i> , 2019, 58, 8735-8738.	1.9	4

#	ARTICLE	IF	CITATIONS
10022	Magnetically Induced Current Densities in Toroidal Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15354-15365.	1.5	20
10023	TriplatinNC and Biomolecules: Building Models Based on Non-covalent Interactions. <i>Frontiers in Chemistry</i> , 2019, 7, 307.	1.8	13
10024	Exploring the electro-optical properties of conjugated polymers based on oligo-selenophene and oligo(3,4-ethylenedioxy-selenophene). <i>Applied Organometallic Chemistry</i> , 2019, 33, e4962.	1.7	4
10025	Topological analysis of CeMn ₅ (M = Co, Rh) electron charge densities. <i>Computational Materials Science</i> , 2019, 164, 205-217.	1.4	3
10026	Visible-Light-Induced Atom Transfer Radical Addition and Cyclization of Perfluoroalkyl Halides with 1,3-Enynes. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 10154-10162.	3.2	82
10027	Ir-catalyzed selective reduction of CO ₂ to the methoxy or formate level with HSiMe(OSiMe ₃) ₂ . <i>Catalysis Science and Technology</i> , 2019, 9, 2858-2867.	2.1	23
10028	Ultrafast photoisomerisation of an isolated retinoid. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10567-10579.	1.3	12
10029	A theoretical investigation of the optoelectronic performance of some new carbazole dyes. <i>Journal of Computational Electronics</i> , 2019, 18, 951-961.	1.3	6
10030	The new metal-based compound from anticancer drug cytarabine: Spectral, electrochemical, DNA-binding, antiproliferative effect and in silico studies. <i>Journal of Molecular Structure</i> , 2019, 1193, 532-543.	1.8	9
10031	Static second-hyperpolarizability of diffuse electron cyclic compounds M ₂ A ₂ (M = Be, Mg, Ca; A = Li, Na, Tl). <i>ETQq</i> 1,1 0.784 1.2	1.2	3
10032	Impact of molecular conformation on transport and transport-related properties at the nanoscale. <i>Applied Surface Science</i> , 2019, 487, 593-600.	3.1	6
10033	Auto-ignition control using an additive with adaptable chemical structure. Part I: Development of a kinetic model for 1,3-cyclohexadiene and 1,3,5-hexatriene combustion. <i>Combustion and Flame</i> , 2019, 205, 466-483.	2.8	13
10034	Synthesis, bioactivities, DFT and in-silico appraisal of azo clubbed benzothiazole derivatives. <i>Journal of Molecular Structure</i> , 2019, 1192, 162-171.	1.8	35
10035	Mössbauer Spectroscopy and Theoretical Studies of Iron Bimetallic Complexes Showing Electrocatalytic Hydrogen Evolution. <i>Inorganic Chemistry</i> , 2019, 58, 7069-7077.	1.9	12
10036	Sigma-holes from iso-molecular electrostatic potential surfaces. <i>Journal of Molecular Modeling</i> , 2019, 25, 160.	0.8	8
10037	Analysis of degradation products of nitrogen mustards via hydrophilic interaction liquid chromatography-tandem mass spectrometry. <i>Journal of Chromatography A</i> , 2019, 1602, 199-205.	1.8	14
10038	Density Functionals from the Multiple-Radii Approach: Analysis and Recovery of the Kinetic Correlation Energy. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3580-3590.	2.3	7
10039	MoCl ₅ as a dual-function redox mediator for Li-O ₂ batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 14239-14243.	5.2	23

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10040	Hole-transporting materials for organic light-emitting diodes: an overview. <i>Journal of Materials Chemistry C</i> , 2019, 7, 7144-7158.	2.7	166
10041	Scalar Relativistic Density Functional Theoretical Investigation of Higher Complexation Ability of Substituted 1,10-Phenanthroline over Bipyridine Towards $\text{Am}^{3+}/\text{Eu}^{3+}$ Ions. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2019, 645, 817-829.	0.6	8
10042	Comparison of spectroscopic, electronic, theoretical, optical and surface morphological properties of functional manganese(III) phthalocyanine compounds for various conditions. <i>Journal of Molecular Structure</i> , 2019, 1193, 247-264.	1.8	14
10043	A "non-dynamical" way of describing room-temperature paramagnetic manganese oxide. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15932-15939.	1.3	6
10044	Uranyl-Bound Tetra-Dentate Non-Innocent Ligands: Prediction of Structure and Redox Behaviour Using Density Functional Theory. <i>ChemPhysChem</i> , 2019, 20, 1869-1878.	1.0	4
10045	Tunable optoelectronic properties of D-A- π -A type dyes by altering auxiliary acceptor position and atomic electronegativity. <i>Journal of Molecular Liquids</i> , 2019, 287, 110883.	2.3	17
10046	Short- and Long-Range Solvation Effects on the Transient UV-Vis Absorption Spectra of a Ru(II)-Polypyridine Complex Disentangled by Nonequilibrium Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2885-2891.	2.1	17
10047	Improved Electro- and Photocatalytic Water Reduction by Confined Cobalt Catalysts in Streptavidin. <i>ACS Catalysis</i> , 2019, 9, 5837-5846.	5.5	28
10048	Triplet exciton diffusion in metalorganic phosphorescent host-guest systems from first principles. <i>Physical Review B</i> , 2019, 99, .	1.1	17
10049	Thermoplastic Aluminoborophosphate-Aniline Polycomplexes. <i>Russian Journal of Physical Chemistry B</i> , 2019, 13, 184-189.	0.2	2
10050	Dual Catalytic Cycle of H ₂ and H ₂ O Oxidations by a Half-Sandwich Iridium Complex: A Theoretical Study. <i>Inorganic Chemistry</i> , 2019, 58, 7274-7284.	1.9	4
10051	A New Member of the BN-Phenanthrene Family: Understanding the Role of the B-N Bond Position. <i>Journal of Organic Chemistry</i> , 2019, 84, 7113-7122.	1.7	23
10052	A first-principles study on the structural, thermal and electronic properties of cerium oxides by using different functionals. <i>Electronic Structure</i> , 2019, 1, 015003.	1.0	6
10053	Cyclization of Terphenyl-Bisfluorenols: A Mechanistic Study of the Regioselectivity. <i>Chemistry - A European Journal</i> , 2019, 25, 10689-10697.	1.7	6
10054	A structural comparative study of charge transfer compounds: Synthesis, crystal structure, IR, Raman-spectroscopy, DFT computation and hirshfeld surface analysis. <i>Journal of Molecular Structure</i> , 2019, 1192, 132-144.	1.8	18
10055	Long-range screened hybrid-functional theory satisfying the local-density linear response. <i>Physical Review A</i> , 2019, 99, .	1.0	16
10056	Nonbonding interaction analyses on PVDF/[BMIM][BF ₄] complex system in gas and solution phase. <i>Journal of Molecular Modeling</i> , 2019, 25, 131.	0.8	21
10057	Nitrogen monoxide storage and sensing applications of transition metal-doped boron nitride nanotubes: a DFT investigation. <i>Structural Chemistry</i> , 2019, 30, 2135-2149.	1.0	9

#	ARTICLE	IF	CITATIONS
10058	Pyridine-2,6-Dicarboxylic Acid Esters (pydicR2) as O,N,O-Pincer Ligands in CuII Complexes. <i>Inorganics</i> , 2019, 7, 53.	1.2	15
10059	Theoretical study of the photophysical processes of a styryl-bodipy derivative eliciting an AND molecular logic gate response. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25958.	1.0	6
10060	Cu ⁺ F Interactions between Cationic Linear N-Heterocyclic Carbene Copper(I) Pyridine Complexes and Their Counterions Greatly Enhance Blue Luminescence Efficiency. <i>Inorganic Chemistry</i> , 2019, 58, 5433-5445.	1.9	52
10061	Homoleptic cis- and trans-palladium(II) bis(guanidinato) complexes derived from N-aryl-N ² ,N ³ -di(pyridin-2-yl)- and N-aryl-N ² ,N ³ -bis(6-methylpyridin-2-yl)guanidines: Catalysts for Heck-Mizoroki coupling reactions. <i>Journal of Organometallic Chemistry</i> , 2019, 892, 1-17.	0.8	4
10062	Gas-Phase Deprotonation of Benzhydryl Cations: Carbene Basicity, Multiplicity, and Rearrangements. <i>Journal of Organic Chemistry</i> , 2019, 84, 7685-7693.	1.7	3
10063	Photochemical mechanism of 1,5-benzodiazepin-2-one: electronic structure calculations and nonadiabatic surface-hopping dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10086-10094.	1.3	15
10064	Active Space Selection Based on Natural Orbital Occupation Numbers from <i>n</i> -Electron Valence Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3522-3536.	2.3	41
10065	Calculation of solvation free energy utilizing a constrained QM/MM approach combined with a theory of solutions. <i>Journal of Chemical Physics</i> , 2019, 150, 114109.	1.2	4
10066	Configuration Space Analysis of the Specific Rotation of Helicenes. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4406-4418.	1.1	9
10067	Catalytic upgrading of ethanol to <i>n</i> -butanol using an aliphatic Mn ^{II} -PNP complex: theoretical insights into reaction mechanisms and product selectivity. <i>Catalysis Science and Technology</i> , 2019, 9, 2794-2805.	2.1	19
10068	Computational simulation and statistical analysis on the relationship between corrosion inhibition efficiency and molecular structure of some hydrazine derivatives in phosphoric acid on mild steel surface. <i>Applied Surface Science</i> , 2019, 491, 707-722.	3.1	106
10069	The Influence of the Electronic Structure Method on Intersystem Crossing Dynamics. The Case of Thioformaldehyde. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3470-3480.	2.3	30
10070	Effect of donor modification on the photo-physical and photo-voltaic properties of N-alkyl/aryl amine based chromophores. <i>New Journal of Chemistry</i> , 2019, 43, 8970-8981.	1.4	17
10071	Impact of fluorination on the photophysics of the flavin chromophore: a quantum chemical perspective. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9912-9923.	1.3	16
10072	Synthesis, optical spectroscopy, structural, and DFT studies on dimeric iodo-bridged Copper(I) complexes. <i>Journal of Organometallic Chemistry</i> , 2019, 892, 75-82.	0.8	3
10073	Enhancement of electronic, photophysical and optical properties of 5,5-Dibromo-2,2-bithiophene molecule: new aspect to molecular design. <i>Opto-electronics Review</i> , 2019, 27, 113-118.	2.4	10
10074	Sub-100 nanometer silver doped gold-cysteine supramolecular assemblies with enhanced nonlinear optical properties. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12091-12099.	1.3	17
10075	Rigidified and expanded N-annulated perylenes as efficient donors in organic sensitizers for application in solar cells. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10488-10496.	1.3	11

#	ARTICLE	IF	CITATIONS
10076	A phosphorescent iridium probe for sensing polarity in the endoplasmic reticulum and <i>in vivo</i> . Dalton Transactions, 2019, 48, 7728-7734.	1.6	11
10077	Molecular Dynamics Simulations on Relaxed Reduced-Dimensional Potential Energy Surfaces. Journal of Physical Chemistry A, 2019, 123, 4543-4554.	1.1	5
10078	Mechanistic insights into a non-heme 2-oxoglutarate-dependent ethylene-forming enzyme: selectivity of ethylene-formation <i>versus</i> Arg hydroxylation. Physical Chemistry Chemical Physics, 2019, 21, 9957-9968.	1.3	40
10079	Molecular Orientation Effects in Organic Light-Emitting Diodes. Helvetica Chimica Acta, 2019, 102, e1900048.	1.0	29
10080	POM-FLPs: [MoIV3] <i>n</i> -polyoxometalate bifunctional catalysis by [MoIV3] <i>n</i> Lewis pairs frustrated by triangular MoIV-MoIV bonds. Dalton Transactions, 2019, 48, 6892-6898.	1.6	14
10081	Investigation of structural ordering in network forming ionic liquids: A molecular dynamics study. Journal of Chemical Physics, 2019, 150, 144904.	1.2	0
10082	One-step synthesis of acriflavine-based carbon dots for adenine detection and a theoretical study on the detection mechanism. Microchemical Journal, 2019, 148, 73-78.	2.3	10
10083	Computer-Aided Design of Luminescent Linear N-Heterocyclic Carbene Copper(I) Pyridine Complexes. Inorganic Chemistry, 2019, 58, 5446-5456.	1.9	35
10084	Vanadyl Porphyrin Speciation Based on Submegahertz Ligand Proton Hyperfine Couplings. Energy & Fuels, 2019, 33, 4237-4243.	2.5	19
10085	Structure-Emission Property Relationships in Cyclometalated Pt(II) η^2 -Diketonate Complexes. Inorganic Chemistry, 2019, 58, 6123-6136.	1.9	24
10086	The impact of the heteroatom in a five-membered ring on the photophysical properties of difluoroborates. Dyes and Pigments, 2019, 170, 107481.	2.0	9
10087	Exploring the Compositional Ternary Diagram of Ge/S/Cu Glasses for Resistance Switching Memories. Journal of Physical Chemistry C, 2019, 123, 9486-9495.	1.5	6
10088	Formation Mechanism of Benzo(a)pyrene: One of the Most Carcinogenic Polycyclic Aromatic Hydrocarbons (PAH). Molecules, 2019, 24, 1040.	1.7	28
10089	CO catalytic oxidation over graphene with double vacancy-embedded molybdenum: a DFT investigation. Carbon Letters, 2019, 29, 337-344.	3.3	8
10090	Synthesis and reactivity at the Ir ^{Me} _{Tpm} platform: from Ir ¹ -N coordination to Ir ³ -N-based organometallic chemistry. Dalton Transactions, 2019, 48, 6455-6463.	1.6	2
10091	The Metal Hydride Problem of Computational Chemistry: Origins and Consequences. Journal of Physical Chemistry A, 2019, 123, 2888-2900.	1.1	26
10092	Sonogashira Cross-Coupling of Aryltrimethylammonium Salts. ACS Catalysis, 2019, 9, 3730-3736.	5.5	43
10093	Modeling Corrosion with First-Principles Electrochemical Phase Diagrams. Annual Review of Materials Research, 2019, 49, 53-77.	4.3	40

#	ARTICLE	IF	CITATIONS
10094	Design and Synthesis of Novel Organic Luminescent Materials Based on Pyrazole Derivative. <i>Journal of Heterocyclic Chemistry</i> , 2019, 56, 1464-1471.	1.4	8
10095	The Electronic Determinants of Spin Crossover Described by Density Functional Theory. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 1-33.	0.6	2
10096	A thiocarbonate sink on the enzymatic energy landscape of aerobic CO oxidation? Answers from DFT and QM/MM models of Mo Cu CO-dehydrogenases. <i>Journal of Catalysis</i> , 2019, 372, 201-205.	3.1	11
10097	Atmospheric Chemistry of Enols: Vinyl Alcohol + OH + O ₂ Reaction Revisited. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3205-3213.	1.1	18
10098	Molecular engineering of anchoring groups for designing efficient triazatruxene-based organic dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2019, 43, 6480-6491.	1.4	15
10099	The UVA response of enolic dibenzoylmethane: beyond the static approach. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 1324-1332.	1.6	9
10100	Rapid synthesis of 4-alkynyl coumarins and tunable electronic properties of emission solvatochromic fluorophores. <i>Dyes and Pigments</i> , 2019, 166, 357-366.	2.0	19
10101	Metal-ligand bifunctional based Mn-catalysts for CO ₂ hydrogenation reaction. <i>Molecular Catalysis</i> , 2019, 468, 109-116.	1.0	15
10102	The basis for reevaluating the reactivity of pyrite surfaces: spin states and crystal field d-orbital splitting energies of bulk, terrace, edge, and corner Fe ions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6415-6431.	1.3	8
10103	Restricted rotation of an Fe(CO) ₂ (PL) ₃ -subunit in [FeFe]-hydrogenase active site mimics by intramolecular ligation. <i>Dalton Transactions</i> , 2019, 48, 5933-5939.	1.6	13
10104	Understanding the spontaneous formation of pyridofuroxan from 2-azido-3-nitropyridine: A theoretical evaluation. <i>Computational and Theoretical Chemistry</i> , 2019, 1154, 31-36.	1.1	1
10105	The correlation factor model for the exchange-correlation energy and its application to transition metal compounds. <i>Journal of Chemical Physics</i> , 2019, 150, 084107.	1.2	10
10106	Theoretical investigation on Ï€-spacer effect of the Ñ€A organic dyes for dye-sensitized solar cell applications: a DFT and TD-BHandH study. <i>Journal of Molecular Modeling</i> , 2019, 25, 92.	0.8	23
10107	Chromo-Fluorogenic Detection of Soman and Its Simulant by Thiourea-Based Rhodamine Probe. <i>Molecules</i> , 2019, 24, 827.	1.7	11
10108	Excited state tracking during the relaxation of coordination compounds. <i>Journal of Computational Chemistry</i> , 2019, 40, 1420-1428.	1.5	12
10109	Functionalized nanoporous gold as a new biosensor platform for ultra-low quantitative detection of human serum albumin. <i>Sensors and Actuators B: Chemical</i> , 2019, 288, 460-468.	4.0	21
10110	Synthesis, DFT/TD-DFT theoretical studies, experimental characterization, electrochemical and antioxidant activity of Fe(III) complexes of bis (dimethylglyoximato) guanine. <i>Journal of Molecular Structure</i> , 2019, 1186, 413-422.	1.8	7
10111	Following local light-induced structure changes and dynamics of the photoreceptor PYP with the thiocyanate IR label. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6622-6634.	1.3	15

#	ARTICLE	IF	CITATIONS
10112	Supramolecularly assisted synthesis of chiral tripodal imidazolium compounds. <i>Organic Chemistry Frontiers</i> , 2019, 6, 1214-1225.	2.3	9
10113	Structural Evolution and Chemical Bonding in Bi-nuclear Niobium Sulfide Clusters: Nb ₂ S _n (n=4-7). <i>Journal of Cluster Science</i> , 2019, 30, 735-746.	1.7	1
10114	Synthesis, characterization, quantum chemical studies and electrochemical performance of new 4,7-dihydro-tetrazolo[1,5-a]pyrimidine derivatives. <i>Journal of Chemical Sciences</i> , 2019, 131, 1.	0.7	6
10115	Can a single water molecule catalyze the OH+CH ₂ CH ₂ and OH+CH ₂ O reactions?. <i>Atmospheric Environment</i> , 2019, 207, 82-92.	1.9	16
10116	Experimental and theoretical study on cetylpyridinium dipicrylamide – A promising ion-exchanger for cetylpyridinium selective electrodes. <i>Journal of Molecular Structure</i> , 2019, 1187, 77-85.	1.8	28
10117	Theoretical investigation of dicarboxamide mono copper (II) and novel transition metal complexes: Structural, chemical reactivity, vibrational and in-silico biological analysis. <i>Journal of Molecular Structure</i> , 2019, 1188, 23-30.	1.8	8
10118	Investigation on bare and hydrogenated Sb-nanosheets as an electrode material for Na-ion battery - A DFT study. <i>Physica B: Condensed Matter</i> , 2019, 562, 75-81.	1.3	33
10119	Density Functional Theory Study of the Capture and Release of Carbon Dioxide by Benzyl Disulfide, Diselenide, and Ditelluride. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3383-3388.	1.1	4
10120	Ligand-centered electrochemical processes enable CO ₂ reduction with a nickel bis(triazapentadienyl) complex. <i>Sustainable Energy and Fuels</i> , 2019, 3, 1172-1181.	2.5	7
10121	Synthesis of novel colorants for DSSC to study effect of alkyl chain length alteration of auxiliary donor on light to current conversion efficiency. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 377, 119-129.	2.0	14
10122	Photocatalytic decarboxylative alkylations mediated by triphenylphosphine and sodium iodide. <i>Science</i> , 2019, 363, 1429-1434.	6.0	520
10123	Rotational Spectrum of Saccharin: Structure and Sweetness. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2756-2761.	1.1	5
10124	Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations Support a Concerted Reaction Mechanism for the Zika Virus NS2B/NS3 Serine Protease with Its Substrate. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2889-2903.	1.2	22
10125	Trifluoromethylation for affecting the structural, electronic and redox properties of cobalt corroles. <i>Dalton Transactions</i> , 2019, 48, 4798-4810.	1.6	28
10126	First-principles calculations of photoluminescence and defect states of C ₃ N ₃ doped		

#	ARTICLE	IF	CITATIONS
10130	Internally Bridged H ₂ Arckel Aromatic [46]Decaphyrins: (Doubly-twisted-Annuleno)Doubly-twisted-Annulene Variants. <i>Chemistry - A European Journal</i> , 2019, 25, 5173-5176.	1.7	4
10131	Electron Delocalization in Planar Metallacycles: H ₂ Arckel or Möbius Aromatic?. <i>ChemistryOpen</i> , 2019, 8, 219-227.	0.9	49
10132	Low-Lying Excited States of hqxCH and Zn-hqxc Complex: Toward Understanding Intramolecular Proton Transfer Emission. <i>Inorganic Chemistry</i> , 2019, 58, 4686-4698.	1.9	10
10133	Cobalt-catalysed unactivated C(sp ³)-H amination: two-state reactivity and multi-reference electronic character. <i>Catalysis Science and Technology</i> , 2019, 9, 1879-1890.	2.1	20
10134	Action-spectroscopy studies of positively charge-tagged azobenzene in solution and in the gas-phase. <i>Journal of Chemical Physics</i> , 2019, 150, 084303.	1.2	1
10135	N-Inversion in N-phenylloxaziridine: substituent and solvent effects via density functional theory. <i>Journal of the Chinese Chemical Society</i> , 2019, 66, 1263-1269.	0.8	0
10136	Excited states and excitonic interactions in prototypic polycyclic aromatic hydrocarbon dimers as models for graphitic interactions in carbon dots. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9077-9088.	1.3	34
10137	Theoretical insights into CO ₂ hydrogenation to methanol by a Mn-PNP complex. <i>Catalysis Science and Technology</i> , 2019, 9, 1867-1878.	2.1	30
10138	Photoprotection assessment of olive (<i>Olea europaea</i> L.) leaves extract standardized to oleuropein: In vitro and in silico approach for improved sunscreens. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2019, 193, 162-171.	1.7	43
10139	Diaminodicyanoquinones: Fluorescent Dyes with High Dipole Moments and Electron-Acceptor Properties. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 8235-8239.	7.2	22
10140	Hydrogen chloride adsorption on large defective PAHs modeling soot surfaces and influence on water trapping: A DFT and AIMD study. <i>Chemical Physics</i> , 2019, 523, 18-27.	0.9	9
10141	TCA self-assembled fluorescence probe for Cu (II) ion based on the unique configuration of extra nuclear electrons of metal ions: A TDDFT study. <i>Computational and Theoretical Chemistry</i> , 2019, 1157, 1-10.	1.1	0
10142	Photochemical Synthesis and Catalytic Applications of Gold Nanoplates Fabricated Using Quercetin Diphosphate Macromolecules. <i>ACS Omega</i> , 2019, 4, 6511-6520.	1.6	12
10143	Game of Isomers: Bifurcation in the Catalytic Formation of Bis[1]benzothieno[1,4]thiazines with Conformation-Dependent Electronic Properties. <i>Journal of Organic Chemistry</i> , 2019, 84, 5582-5595.	1.7	6
10144	Functionalized 2-hydrazinobenzothiazole with carbohydrates as a corrosion inhibitor: electrochemical, XPS, DFT and Monte Carlo simulation studies. <i>Materials Chemistry Frontiers</i> , 2019, 3, 931-940.	3.2	66
10145	Diaminodicyanochinone - Fluoreszenzfarbstoffe mit hohem Dipolmoment und Elektronenakzeptoreigenschaften. <i>Angewandte Chemie</i> , 2019, 131, 8321-8326.	1.6	2
10146	Surface-enhanced Raman scattering based sensing of trans-urocanic acid, an epidermal photoreceptor using silver nanoparticles aided by density functional theoretical calculations. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 837-846.	1.2	15
10147	Computational ¹ H NMR: Part 1. Theoretical background. <i>Magnetic Resonance in Chemistry</i> , 2019, 57, 897-914.	1.1	44

#	ARTICLE	IF	CITATIONS
10148	New blue light emitting cyanopyridine based conjugated polymers: From molecular engineering to PLED applications. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 378, 38-45.	2.0	19
10149	Characterization of electrophilicity and oxidative potential of atmospheric carbonyls. <i>Environmental Sciences: Processes and Impacts</i> , 2019, 21, 856-866.	1.7	17
10150	Investigation of spectroscopic studies and DFT calculations on glucofuranose derivatives of dithiophosphonates. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2019, 194, 1054-1061.	0.8	2
10151	High-Temperature Cooperative Spin Crossover Transitions and Single-Crystal Reflection Spectra of [FeII(qsal)2](CH3OSO3) and Related Compounds. <i>Crystals</i> , 2019, 9, 81.	1.0	11
10152	Complexes of Hyperguinones A and B with a Cu ²⁺ Ion. <i>Advances in Quantum Chemistry</i> , 2019, 78, 83-108.	0.4	10
10153	Long Carbon-Based Chains of Interstellar Medium Can Have a Triplet Ground State. Why Is This Important for Astrochemistry?. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 863-872.	1.2	18
10154	[Cr(tpy)2] ³⁺ as a multi-electron reservoir for photoinduced charge accumulation. <i>Dalton Transactions</i> , 2019, 48, 6800-6811.	1.6	12
10155	Synthesis and Characterization of a Molecularly Designed High-Performance Organodisulfide as Cathode Material for Lithium Batteries. <i>Advanced Energy Materials</i> , 2019, 9, 1900705.	10.2	34
10156	Fully numerical Hartree-Fock and density functional calculations. I. Atoms. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25945.	1.0	26
10157	Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchange-Correlation Functionals: The MOBH35 Benchmark Database. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3761-3781.	1.1	104
10158	Tellurorhodamine photocatalyzed aerobic oxidation of organo-silanes and phosphines by visible-light. <i>Dalton Transactions</i> , 2019, 48, 5665-5673.	1.6	16
10159	Cerium(IV) based oxidative free radical cyclization of active methylene compounds with some cyclic alkenes: A useful annulation method for terpene functionalization. <i>Tetrahedron</i> , 2019, 75, 2652-2663.	1.0	4
10160	The mechanism of the gold-catalyzed intramolecular [3 + 2]-cycloaddition of 1,6-diyne: a DFT study. <i>Dalton Transactions</i> , 2019, 48, 5698-5704.	1.6	4
10161	High-level theoretical benchmark investigations of the UV-vis absorption spectra of paradigmatic polycyclic aromatic hydrocarbons as models for graphene quantum dots. <i>Journal of Chemical Physics</i> , 2019, 150, 124302.	1.2	35
10162	Understanding the effect of thionation on naphthalene diimide using first-principles predictions of near-edge x-ray absorption fine structure spectra. <i>Journal of Chemical Physics</i> , 2019, 150, 104302.	1.2	4
10163	Conformationally Rigid Ethynylene-Cumulene Conjugated Aromatic [30] Heteroannulenes with NIR Absorption: Synthesis, Spectroscopic and Theoretical Characterization. <i>Journal of Organic Chemistry</i> , 2019, 84, 5203-5212.	1.7	7
10164	A quantum chemical study of the effect of substituents in governing the strength of the S-F bonds of sulfenyl-type fluorides toward homolytic dissociation and fluorine atom transfer. <i>Chemical Data Collections</i> , 2019, 20, 100186.	1.1	5
10165	Computational Modelling Study on the Pseudoazurin Type Cu Site. , 2019, , .		0

#	ARTICLE	IF	CITATIONS
10166	A greener catalyst for hydroboration of imines—external electric field modify the reaction mechanism. <i>Journal of Computational Chemistry</i> , 2019, 40, 1772-1779.	1.5	11
10167	How does Mo-dependent perchlorate reductase work in the decomposition of oxyanions?. <i>Dalton Transactions</i> , 2019, 48, 5683-5691.	1.6	11
10168	Cysteine Modified by S-Sulfation: Consequence on Fragmentation Processes Elucidated by Tandem Mass Spectrometry and Chemical Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3685-3696.	1.1	20
10169	From Alkane to Alkene: The Inert Aliphatic C-H Bond Activation Presented by Binuclear Iron Stearoyl-CoA Desaturase with a Long di-Fe Distance of 6 Å.... <i>ACS Catalysis</i> , 2019, 9, 4345-4359.	5.5	8
10170	Efficient electron transfer across hydrogen bond interfaces by proton-coupled and -uncoupled pathways. <i>Nature Communications</i> , 2019, 10, 1531.	5.8	42
10171	Types of Six-Membered N-Heterocyclic Germanium Radicals: A Combined Computational and Experimental Study. <i>Inorganic Chemistry</i> , 2019, 58, 5688-5694.	1.9	11
10172	Do An(III) and Ln(III) ions form heteroleptic complexes with diglycolamide and hydrophilic BT(B)P ligands in solvent extraction systems? A spectroscopic and DFT study. <i>New Journal of Chemistry</i> , 2019, 43, 6314-6322.	1.4	12
10173	Cyclobutyne: Minimum or Transition State?. <i>Journal of Organic Chemistry</i> , 2019, 84, 5548-5553.	1.7	3
10174	Projector-Based Embedding Eliminates Density Functional Dependence for QM/MM Calculations of Reactions in Enzymes and Solution. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2063-2078.	2.5	27
10175	Adsorption Study of Al ³⁺ , Cr ³⁺ , and Mn ²⁺ onto Quartz and Corundum using Flow Microcalorimetry, Quartz Crystal Microbalance, and Density Functional Theory. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 432-441.	1.2	16
10176	Computational modeling of curcumin-based fluorescent probe molecules. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	3
10177	Amino acids-clay interaction at the nano-atomic scale: The l-alanine-chlorite system. <i>Applied Clay Science</i> , 2019, 172, 28-39.	2.6	13
10178	Dicyanamide-interlaced assembly of Zn(II)-schiff-base complexes derived from salicylaldimino type compartmental ligands: Syntheses, crystal structures, FMO, ESP, TD-DFT, fluorescence lifetime, in vitro antibacterial and anti-biofilm properties. <i>Inorganica Chimica Acta</i> , 2019, 489, 244-254.	1.2	49
10179	Synthesis of red emitting triphenylamine derived NLOphoric D-π-A molecules: photophysical, and viscosity sensing studies. <i>SN Applied Sciences</i> , 2019, 1, 1.	1.5	6
10180	Recent advances in computational photocatalysis: A review. <i>Canadian Journal of Chemical Engineering</i> , 2019, 97, 1982-1998.	0.9	45
10181	Mechanistic Insights into the Reaction of N-Propargylated Pyrrole and Indole Carbaldehyde with Ammonia, Alkyl Amines, and Branched Amines: A Synthetic and Theoretical Investigation. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 5261-5274.	1.2	15
10182	The planarity of heteroatom analogues of benzene: Energy component analysis and the planarization of hexasilabenzene. <i>Journal of Computational Chemistry</i> , 2019, 40, 581-590.	1.5	7
10183	The Perlin effect in 2-halocyclohexanones and 2-halocyclohexanethiones. <i>Computational and Theoretical Chemistry</i> , 2019, 1152, 28-31.	1.1	2

#	ARTICLE	IF	CITATIONS
10184	Different elements doped graphene sensor for CO ₂ greenhouse gases detection: The DFT study. <i>Chemical Physics Letters</i> , 2019, 721, 33-37.	1.2	57
10185	Pyridine-2-carboxylato chelated acylrhodium(III) organometallics: Spectroscopic, structural and theoretical studies. <i>Polyhedron</i> , 2019, 172, 15-21.	1.0	1
10186	A Consistent Reduced Network for HCN Chemistry in Early Earth and Titan Atmospheres: Quantum Calculations of Reaction Rate Coefficients. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1861-1873.	1.1	15
10187	Impact of heteroatom (S and N) position and change in central ring of anthracene with heterocyclic ring on charge transport and optical properties in anthratetrathiazole (ATTz). <i>Journal of Sulfur Chemistry</i> , 2019, 40, 361-376.	1.0	4
10188	Identifying absolute configurations of PCB atropisomers by comparison of their experimental specific rotations with their DFT calculated values. <i>Canadian Journal of Chemistry</i> , 2019, 97, 325-330.	0.6	2
10189	Understanding the adsorption of Pb ²⁺ , Hg ²⁺ and Zn ²⁺ from aqueous solution on a lignocellulosic biomass char using advanced statistical physics models and density functional theory simulations. <i>Chemical Engineering Journal</i> , 2019, 365, 305-316.	6.6	94
10190	D-A- π -A based organic dyes for efficient DSSCs: A theoretical study on the role of π -spacer. <i>Computational Materials Science</i> , 2019, 161, 163-176.	1.4	65
10191	DFT computational schemes for ¹⁵ N NMR chemical shifts of the condensed nitrogen-containing heterocycles. <i>Magnetic Resonance in Chemistry</i> , 2019, 57, 346-358.	1.1	7
10192	A probe into underlying factors affecting ultrafast charge transfer at Donor/IDIC interface of all-small-molecule nonfullerene organic solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 375, 1-8.	2.0	11
10193	Exciplex Stabilization in Asymmetric Acene Dimers. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1796-1806.	1.1	13
10194	Partial combination of composite strategy and the B3LYP functional for the calculation of enthalpies of formation. <i>Journal of Molecular Modeling</i> , 2019, 25, 62.	0.8	8
10195	Terahertz spectroscopy of diglycidylether of bisphenol A: Experimental investigations and density functional theory based simulations. <i>Journal of Molecular Structure</i> , 2019, 1184, 114-122.	1.8	7
10196	Computational study of acylphloroglucinols: an investigation with many branches. <i>Pure and Applied Chemistry</i> , 2019, 91, 597-607.	0.9	7
10197	Effect of Nuclear Motion on Charge Transport in Fullerenes: A Combined Density Functional Tight Binding-Density Functional Theory Investigation. <i>Frontiers in Energy Research</i> , 2019, 7, .	1.2	9
10198	Sequential Cu-catalyzed Four- and Five-Component Syntheses of Luminescent 3-Triazolylquinoxalines. <i>Chemistry - A European Journal</i> , 2019, 25, 9447-9455.	1.7	13
10199	Synthesis and Characterization of [Br ₃][MF ₆] (M=Sb, Ir), as well as Quantum Chemical Study of [Br ₃] ⁻ + Structure, Chemical Bonding, and Relativistic Effects Compared with [XBr ₂] ⁻ + (X=Br, I, At, Ts) and [TsZ ₂] ⁻ + (Z=F, Cl, Br, I, At, Ts). <i>Chemistry - A European Journal</i> , 2019, 25, 5793-5802.	1.7	10
10200	Theoretical Studies on Hexanuclear [M ₃ (μ_4 -O/OH)] ₂ (M = Fe(III), Tj ETQq0 0 0 rgBT/Overlock Correlations. <i>Inorganic Chemistry</i> , 2019, 58, 3175-3188.	1.9	27
10201	Efficient HF exchange evaluation through Fourier convolution in Cartesian grid for orbital-dependent density functionals. <i>Journal of Chemical Physics</i> , 2019, 150, 064104.	1.2	6

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10202	Theoretical Surface Science Beyond Gradient-Corrected Density Functional Theory: Water at $\sqrt{2} \times \sqrt{3}$ (0001) as a Case Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6675-6684.	1.5	15
10203	First-Principles Investigation of Adsorption of Ag on Defected and Ce-doped Graphene. <i>Materials</i> , 2019, 12, 649.	1.3	9
10204	Comparing the Self-Assembly of Sexiphenyl-Dicarbonitrile on Graphite and Graphene on Cu(111). <i>Chemistry - A European Journal</i> , 2019, 25, 5065-5070.	1.7	4
10205	Dual level direct dynamics study of gas phase reaction of $\text{CF}_3\text{CH}_2\text{OCH}_2\text{CF}_3$ with Cl atoms and atmospheric degradation of $\text{CF}_3\text{CH}_2\text{OCH}_2\text{CF}_3$. <i>Chemical Physics Letters</i> , 2019, 721, 141-148.	1.2	6
10206	A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User. <i>Australian Journal of Chemistry</i> , 2019, 72, 563.	0.5	115
10207	Experimental and Theoretical Studies of Trisodium-1,3,5-Benzene Tricarboxylate as a Low-Voltage Anode Material for Sodium-Ion Batteries. <i>Energy Technology</i> , 2019, 7, 1801030.	1.8	13
10208	Stability, electronic and optical properties of the boron nitride cage (B ₄₇ N ₅₃) from quantum mechanical calculations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 111, 118-126.	1.3	23
10209	From Mechanistic Investigation to Quantitative Prediction. , 2019, , 287-326.		4
10210	Scalable and safe synthetic organic electroreduction inspired by Li-ion battery chemistry. <i>Science</i> , 2019, 363, 838-845.	6.0	305
10211	Small Polarons in Transition Metal Oxides. , 2019, , 1-39.		20
10212	Evolution of local atomic structure during solidification of U ₁₁₆ Nb ₁₂ liquid: An ab initio molecular dynamics study. <i>Journal of Alloys and Compounds</i> , 2019, 787, 267-275.	2.8	14
10213	Carbon monoxide adsorption at forsterite surfaces as models of interstellar dust grains: An unexpected bathochromic (red) shift of the CO stretching frequency. <i>Journal of Chemical Physics</i> , 2019, 150, 064702.	1.2	4
10214	Space partitioning of exchange-correlation functionals with the projector augmented-wave method. <i>Journal of Chemical Physics</i> , 2019, 150, 054101.	1.2	8
10215	A new tripodal kojic acid derivative for iron sequestration: Synthesis, protonation, complex formation studies with Fe ³⁺ , Al ³⁺ , Cu ²⁺ and Zn ²⁺ , and in vivo bioassays. <i>Journal of Inorganic Biochemistry</i> , 2019, 193, 152-165.	1.5	22
10216	Catalyst-Dependent Chemoselectivity in the Dirhodium-Catalyzed Cyclization Reactions Between Enodiazacetamide and Nitrosoarene: A Theoretical Study. <i>Frontiers in Chemistry</i> , 2019, 7, 586.	1.8	6
10217	Structural and Electronic Properties of B ₈ , VB ₈ , CRB ₈ , and MNB ₈ Nanoclusters: A DFT study. , 2019, , .		0
10218	First Principle Study of Pristine and Zn Doped B ₆ Nanocluster. , 2019, , .		1
10219	A Novel Ruthenium(II) Polypyridyl Complex Bearing 1,8-Naphthyridine as a High Selectivity and Sensitivity Fluorescent Chemosensor for Cu ²⁺ and Fe ³⁺ Ions. <i>Molecules</i> , 2019, 24, 4032.	1.7	6

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10220	Coordination of 2,2,2-(Trifluoroazanediy)bis(<i>N,N</i> -dimethylacetamide) with U(VI), Nd(III), and Np(V): A Thermodynamic and Structural Study. <i>Inorganic Chemistry</i> , 2019, 58, 15962-15970.	1.9	10
10221	Dispersion-driven conformational preference in the gas phase: Microwave spectroscopic and theoretical study of allyl isocyanate. <i>Journal of Chemical Physics</i> , 2019, 151, 194304.	1.2	6
10222	Direct arylation of heteroarenes by PEPPSI-type palladium-NHC complexes and representative quantum chemical calculations for the compound which the structure was determined by X-ray crystallography. <i>Journal of Coordination Chemistry</i> , 2019, 72, 3258-3284.	0.8	9
10223	Investigating Charge Transfer Interactions in AuCe ₂ O _n Clusters Using Photoionization Efficiency Spectroscopy and Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10158-10168.	1.1	7
10224	A Comparative Computational Study of the Adsorption of TCNQ and F4-TCNQ on the Coinage Metal Surfaces. <i>ACS Omega</i> , 2019, 4, 16906-16915.	1.6	9
10225	Some observations on the performance of the most recent exchange-correlation functionals for the large and chemically diverse GMTKN55 benchmark. <i>AIP Conference Proceedings</i> , 2019, , .	0.3	15
10226	Distinct ionic adsorption sites in defective Prussian blue: a 3D-RISM study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22569-22576.	1.3	6
10227	The control effects of different scaffolds in chiral phosphoric acids: a case study of enantioselective asymmetric arylation. <i>Catalysis Science and Technology</i> , 2019, 9, 6482-6491.	2.1	7
10228	Theoretical investigation of the mechanism, kinetics and subsequent degradation products of the NO ₃ radical initiated oxidation of 4-hydroxy-3-hexanone. <i>Environmental Sciences: Processes and Impacts</i> , 2019, 21, 2080-2092.	1.7	0
10229	Expanstines A-D: four unusual isoprenoid epoxy cyclohexenones generated by <i>Penicillium expansum</i> -15 fermentation and photopromotion. <i>Organic Chemistry Frontiers</i> , 2019, 6, 3839-3846.	2.3	19
10230	Improving LMOF luminescence quantum yield through guest-mediated rigidification. <i>Journal of Materials Chemistry C</i> , 2019, 7, 14739-14744.	2.7	17
10231	The simulation of X-ray absorption spectra from ground and excited electronic states using core-valence separated DFT/MRCl. <i>Journal of Chemical Physics</i> , 2019, 151, 144104.	1.2	19
10232	Adiabatic connection in density functional theory in two-dimensions: A semi-analytic wavefunction based study for two-electron atomic systems. <i>Journal of Chemical Physics</i> , 2019, 151, 204104.	1.2	1
10233	Non-linear optical properties of carbazole based dyes modified with diverse spacer units for dye-sensitized solar cells: A first principle study. <i>AIP Conference Proceedings</i> , 2019, , .	0.3	1
10234	¹³ C- ¹³ C spin-coupling constants in crystalline ¹³ C-labeled saccharides: conformational effects interrogated by solid-state ¹³ C NMR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23576-23588.	1.3	9
10235	How carotenoid distortions may determine optical properties: lessons from the Orange Carotenoid Protein. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23187-23197.	1.3	23
10236	Lanthanide and actinide doped B ₁₂ H ₁₂ ²⁺ and Al ₁₂ H ₁₂ ²⁺ clusters: new magnetic superatoms with f-block elements. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23720-23732.	1.3	5
10237	Ab initio dynamics of hydrogen abstraction from N ₂ H ₄ by OH radicals: an RRKM-based master equation study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23733-23741.	1.3	12

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10238	Theoretical study of aromatic hydroxylation of the [Cu ₂ (H-XYL)O ₂] ²⁺ complex mediated by a side-on peroxo dicopper core and Cu-ligand effects. <i>Dalton Transactions</i> , 2019, 48, 16882-16893.	1.6	1
10239	Origins of stereoselectivity in uncatalyzed and ZnBr ₂ -catalyzed Diels-Alder reactions of a chiral sulfinylquinone. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 8756-8767.	1.5	0
10240	Systematic characterisation of the structure and radical scavenging potency of Pu'Er tea () polyphenol theaflavin. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 9942-9950.	1.5	11
10241	The decomposition mechanism of C ₄ F ₇ N-Cu gas mixtures. <i>AIP Advances</i> , 2019, 9, .	0.6	5
10242	Conformational Equilibria and Molecular Structures of Model Sulfur-Sulfur Bridge Systems: Diisopropyl Disulfide. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10714-10720.	1.1	5
10243	Molecular Docking of a Bio Material [1-[[<i>Z</i> -Cyclopentylidene] Amino]-3-Phenylthiourea] by First Principles Study. <i>Polycyclic Aromatic Compounds</i> , 2021, 41, 1667-1680.	1.4	3
10244	Photoelectron spectroscopy of [Mo ₆ X ₁₄] ²⁻ dianions (X = Cl ⁻ , I ⁻). <i>Journal of Chemical Physics</i> , 2019, 151, 194310.	1.2	3
10245	Computational and experimental assessment on the nonlinear optical properties of platinum(II) arylacetylides with donor-acceptor structures. <i>Journal of Organometallic Chemistry</i> , 2019, 904, 121003.	0.8	3
10246	Anti-inflammatory diterpenoids from the Brazilian alga <i>Dictyota menstrualis</i> . <i>Algal Research</i> , 2019, 44, 101695.	2.4	4
10247	Mechanochemical Improvement of Norbornadiene-Based Molecular Solar-Thermal Systems Performance. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 19496-19504.	3.2	10
10248	Cl Atoms and OH Radicals Initiated Kinetic and Mechanistic Study on the Degradation of Propyl Butanoate under Tropospheric Conditions. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10976-10989.	1.1	5
10249	Density Functional Theory Studies on Zeolitic Imidazolate Framework-8 and Ionic Liquid-Based Composite Materials. <i>ACS Omega</i> , 2019, 4, 22655-22666.	1.6	21
10250	Systematic beyond-DFT study of binary transition metal oxides. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	50
10251	Synthesis, spectroscopic (FT-IR and UV-Vis), crystallographic and theoretical studies, and a molecular docking simulation of an imatinib-like template. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 1681-1689.	0.2	2
10252	(3 <i>S</i> ,4 <i>R</i>)-3,4-Dihydroxy-N-alkyl-l-homoprolines: synthesis and computational mechanistic studies. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 10052-10064.	1.5	1
10253	Excess electron solvation in ammonia clusters. <i>Journal of Chemical Physics</i> , 2019, 151, 204304.	1.2	13
10254	Controllable catalytic difluorocarbene transfer enables access to diversified fluoroalkylated arenes. <i>Nature Chemistry</i> , 2019, 11, 948-956.	6.6	125
10255	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. <i>Journal of Chemical Physics</i> , 2019, 151, 214108.	1.2	56

#	ARTICLE	IF	CITATIONS
10256	Mediation of Electron Transfer by Quadrupolar Interactions: The Constitutional, Electronic, and Energetic Complementarities in Supramolecular Chemistry. <i>IScience</i> , 2019, 22, 269-287.	1.9	7
10257	Isomeric Ir(III) complexes for tracking mitochondrial pH fluctuations and inducing mitochondrial dysfunction during photodynamic therapy. <i>Dalton Transactions</i> , 2019, 48, 17200-17209.	1.6	16
10258	Thermoelectric properties of heavy fermion CeRhIn5 using density functional theory combined with semiclassical Boltzmann theory. <i>RSC Advances</i> , 2019, 9, 36182-36197.	1.7	6
10259	A model for dinitrogen binding in the E ₄ state of nitrogenase. <i>Chemical Science</i> , 2019, 10, 11110-11124.	3.7	48
10260	Synthesis, DFT studies and photovoltaic characteristics of 2-amino-N-cyclohexyl-5-oxo-5H-chromeno[2,3-b]pyridine-3-carboxamide (ACCP). <i>Applied Surface Science</i> , 2019, 467-468, 1226-1238.	3.1	12
10261	Mechanistic Insights into the Electrochemical Reduction of CO ₂ Catalyzed by Iron Cyclopentadienone Complexes. <i>Organometallics</i> , 2019, 38, 1236-1247.	1.1	23
10262	Catalytic oxidation mechanisms of carbon monoxide over single and double vacancy Cr-embedded graphene. <i>Journal of Materials Science</i> , 2019, 54, 1395-1408.	1.7	11
10263	Synthesis and emissive properties of bi-directed azomethine iron(III) complexes based on salicylidene-4-biphenylcarboxylic acid. <i>Journal of Molecular Structure</i> , 2019, 1176, 529-537.	1.8	5
10264	Quantum Monte Carlo assessment of density functionals for π -electron molecules: ethylene and bifuran. <i>Molecular Physics</i> , 2019, 117, 2241-2250.	0.8	1
10265	Microwave-assisted Synthesis, Characterization, and Density Functional Theory Study of Biologically Active Ferrocenyl Bis-pyrazoline and Bis-pyrimidine as Organometallic Macromolecules. <i>Journal of Heterocyclic Chemistry</i> , 2019, 56, 312-318.	1.4	20
10266	Aromatic Pathways in Porphycene Derivatives Based on Current-Density Calculations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 284-292.	1.1	1
10267	Employing broken symmetry effects from unrestricted coupled cluster wave function to determine dynamic and non-dynamic electron correlation during triple bond breaking in the N ₂ molecule. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25865.	1.0	2
10268	On the molecular origin of the sensitivity to impact of cyclic nitramines. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25868.	1.0	16
10269	Density functionals for nondynamical correlation constructed from an upper bound to the exact exchange energy density. <i>Molecular Physics</i> , 2019, 117, 1226-1241.	0.8	8
10270	Developing Consistent Molecular Dynamics Force Fields for Biological Chromophores via Force Matching. <i>Journal of Physical Chemistry B</i> , 2019, 123, 428-438.	1.2	21
10271	Spectroscopic and Computational Evidence of Intramolecular Au ^I ...H ⁺ ...N Hydrogen Bonding. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 2011-2016.	7.2	51
10272	Bis[1]benzothieno[1,4]thiazines: Planarity, Enhanced Redox Activity and Luminescence by Thieno-Expansion of Phenothiazine. <i>Chemistry - A European Journal</i> , 2019, 25, 3582-3590.	1.7	12
10273	Manganese (II) complexes containing carbacylamidophosphate ligands: Synthesis, molecular structures and computational investigation. <i>Journal of Molecular Structure</i> , 2019, 1181, 61-70.	1.8	0

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10274	Spectroscopic, structural, electrochemical, and cytotoxicity studies on dithiocarbamate-chelated ruthenium organometallics incorporating imine-phenol function. <i>Journal of Coordination Chemistry</i> , 2019, 72, 180-200.	0.8	6
10275	Electronic Coupling and Electron Transfer between Two Mo ₂ Units through <i>meta</i> - and <i>para</i> -Phenylene Bridges. <i>Chemistry - A European Journal</i> , 2019, 25, 3930-3938.	1.7	18
10276	Benchmark study of popular density functionals for calculating binding energies of three-center two-electron bonds. <i>Journal of Computational Chemistry</i> , 2019, 40, 657-670.	1.5	11
10277	Stabilizing Borinium Cations [X ⁺ B ⁺ X ⁺] through Conjugation and Hyperconjugation Effects. <i>Inorganic Chemistry</i> , 2019, 58, 243-249.	1.9	2
10278	Matched/Mismatched Cases in Proline-Catalyzed Cascade Reactions with Carbohydrates: A Computational Insight into the Role of <i>d</i> - and <i>l</i> -Proline. <i>Journal of Organic Chemistry</i> , 2019, 84, 1201-1217.	1.7	5
10279	Lone pairs vs. covalent bonds: conformational effects in bicyclo[3.3.1]nonane derivatives. <i>Structural Chemistry</i> , 2019, 30, 509-522.	1.0	7
10280	High level ab initio thermochemistry of SF ₅ OOO radical. <i>Computational and Theoretical Chemistry</i> , 2019, 1148, 8-15.	1.1	2
10281	Insights into the crystal size and morphology of photocatalysts. <i>Journal of Colloid and Interface Science</i> , 2019, 538, 638-647.	5.0	22
10282	Evaluating Density Functionals by Examining Molecular Structures, Chemical Bonding, and Relative Energies of Mononuclear Ru ^{II} -Cl ⁻ -H ⁻ -PR ₃ Isomers. <i>Journal of Physical Chemistry A</i> , 2019, 123, 343-358.	1.1	1
10283	Synthesis, characterisation, estimation of ground-and excited-state dipole moments using solvatochromic shift and theoretical studies of new iminocoumarin derivatives. <i>Journal of Molecular Structure</i> , 2019, 1181, 270-278.	1.8	3
10284	Photophysics of OLED Materials with Emitters Exhibiting Thermally Activated Delayed Fluorescence and Used in Hole/Electron Transporting Layer from Optimally Tuned Range-Separated Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2019, 123, 746-761.	1.5	18
10285	Uncatalyzed gas phase aziridination of alkenes by organic azides. Part 2. Whole azide reaction with alkene. <i>Journal of Chemical Sciences</i> , 2019, 131, 1.	0.7	5
10286	Synthesis of tetra-substituted phthalocyanines bearing 2-(ethyl(<i>m</i> -tolyl)amino)ethanol: Computational and photophysicochemical studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 373, 77-86.	2.0	31
10287	Gas-Phase Ozone Reactions with a Structurally Diverse Set of Molecules: Barrier Heights and Reaction Energies Evaluated by Coupled Cluster and Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 517-536.	1.1	13
10288	Solvent-Controlled CO ₂ Reduction by a Triphos ⁻ Iron Hydride Complex. <i>Organometallics</i> , 2019, 38, 289-299.	1.1	17
10289	Cucurbit[7]uril-Carbazole Two-Photon Photoinitiators for the Fabrication of Biocompatible Three-Dimensional Hydrogel Scaffolds by Laser Direct Writing in Aqueous Solutions. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 1782-1789.	4.0	52
10290	Through-space spin-spin coupling constants involving fluorine: benchmarking DFT functionals. <i>Molecular Physics</i> , 2019, 117, 1469-1480.	0.8	18
10291	Study on the binding mode of a pyrrolotriazin derivative with JAK2 by docking and MD simulation. <i>Molecular Simulation</i> , 2019, 45, 230-238.	0.9	1

#	ARTICLE	IF	CITATIONS
10292	Photophysical Impact of Diacetylenic Conjugation on Classical Donor–Acceptor Electronic Energy Pair. <i>Journal of Physical Chemistry A</i> , 2019, 123, 443-453.	1.1	6
10293	Germanene nanosheets as a novel anode material for sodium-ion batteries—a first-principles investigation. <i>Materials Research Express</i> , 2019, 6, 035504.	0.8	30
10294	How Does Vibrational Excitation Affect the X-Ray Absorption Spectra of Monohydrated Halide and Alkali Metal Clusters?. <i>Advances in Quantum Chemistry</i> , 2019, , 57-81.	0.4	0
10295	Dynamical and Environmental Effects on the Optical Properties of an Heteroleptic Ru(II)–Polypyridine Complex: A Multilevel Approach Combining Accurate Ground and Excited State QM-Derived Force Fields, MD and TD-DFT. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 529-545.	2.3	17
10296	DFT and TD-DFT calculations on thieno[2,3-b]indole-based compounds for application in organic bulk heterojunction (BHJ) solar cells. <i>Research on Chemical Intermediates</i> , 2019, 45, 1327-1340.	1.3	8
10297	Adsorption for SO ₂ gas molecules on B, N, P and Al doped MoS ₂ : The DFT study. <i>Chemical Physics Letters</i> , 2019, 715, 273-277.	1.2	41
10298	[8] Cyclo-1, 4-naphthylene: A possible new member in hole transport family. <i>Chemical Physics Letters</i> , 2019, 715, 153-159.	1.2	2
10299	Synthesis of tetra-substituted metallophthalocyanines: Spectral, structural, computational studies and investigation of their photophysical and photochemical properties. <i>Polyhedron</i> , 2019, 158, 316-324.	1.0	28
10300	Highly fluorescent materials derived from ortho-vanillin: Structural, photophysical electrochemical and theoretical studies. <i>Journal of Molecular Liquids</i> , 2019, 275, 792-806.	2.3	13
10301	Synthesis, characterization, theoretical studies, ADMET and drug-Likeness analysis: Electrochemical and biological activities of metal complexes of 3-(2-hydroxybenzoyl)-2H-chromen-2-one. <i>Journal of Molecular Structure</i> , 2019, 1179, 495-505.	1.8	21
10302	Crystallographic, spectroscopic and theoretical investigations on Ni(II) complexes of a tridentate NNS donor thiosemicarbazone. <i>Polyhedron</i> , 2019, 158, 398-407.	1.0	14
10303	Estimation of maximum absorption wavelength of polymethine dyes in visible and near-infrared region based on time-dependent density functional theory. <i>Chemical Physics</i> , 2019, 518, 15-24.	0.9	15
10304	Spectroscopic and theoretical studies of some 2-(methoxy)-[(4-substituted)-phenylsulfanyl]-4-(2-substituted) acetophenones. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 210, 82-97.	2.0	4
10305	A new mechanistic insight of DNA base adenine formation from pentamer HCN in the gas phase of interstellar clouds. <i>Journal of Taibah University for Science</i> , 2019, 13, 105-111.	1.1	7
10306	A molecular modelling study of the effects of pivalate ligand substitutions on the magnetic properties of chromium-wheels host complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 87, 41-47.	1.3	1
10307	Room temperature helical fluids in single-component systems. <i>Journal of Molecular Liquids</i> , 2019, 275, 849-858.	2.3	7
10308	Syntheses, crystal structures and photo physical aspects of azido-bridged tetranuclear cadmium (II) complexes: DFT/TD-DFT, thermal, antibacterial and anti-biofilm properties. <i>Journal of Molecular Structure</i> , 2019, 1179, 694-708.	1.8	27
10309	A bonding evolution theory study on the catalytic Noyori hydrogenation reaction. <i>Molecular Physics</i> , 2019, 117, 1315-1324.	0.8	14

#	ARTICLE	IF	CITATIONS
10310	On the Stability of Disubstituted Cyclobutenes – A Computational Study. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 338-341.	1.2	7
10311	Cycloaddition Reaction of Mesoionic 4-Trifluoroacetyl-1,3-oxazolium Salts with Enamines Affording 2-Trifluoroacetylpyrroles. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 1535-1541.	1.2	6
10312	Synthesis of 2-methyl-5-(5-phenyl substituted-1,3,4 oxadiazole-2-yl) quinazolin-4-one fluorescent brightening agent: Computational and experimental comparison of photophysical structure. <i>Journal of Molecular Structure</i> , 2019, 1182, 150-157.	1.8	5
10313	A problem in the structure assignment of acremolin C, which is most probably identical with acremolin B. <i>Natural Product Research</i> , 2019, 33, 3011-3015.	1.0	5
10314	Triplet Tuning: A Novel Family of Non-Empirical Exchange-Correlation Functionals. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1226-1241.	2.3	34
10315	Synthesis, antioxidant activity and SAR study of novel spiro-isatin-based Schiff bases. <i>Molecular Diversity</i> , 2019, 23, 829-844.	2.1	52
10316	Theoretical study of the effects of modifying the structures of organic dyes based on N,N-alkylamine on their efficiencies as DSSC sensitizers. <i>Journal of Molecular Modeling</i> , 2019, 25, 9.	0.8	20
10317	Design, synthesis, antimicrobial activity and computational studies of novel azo linked substituted benzimidazole, benzoxazole and benzothiazole derivatives. <i>Computational Biology and Chemistry</i> , 2019, 78, 330-337.	1.1	98
10318	Pyridine-2-olato chelated ruthenium(II) organometallics incorporating imine-phenol function: spectroscopic, structural, electrochemical, and theoretical studies. <i>Journal of Coordination Chemistry</i> , 2019, 72, 164-179.	0.8	2
10319	Monomeric zinc(II) amide complexes supported by bidentate, benzannulated phenanthridine amido ligands. <i>Polyhedron</i> , 2019, 161, 261-267.	1.0	13
10320	Complexes formed by the siderophore-based monosulfactam antibiotic BAL30072 and their interaction with the outer membrane receptor PiuA of <i>P. aeruginosa</i> . <i>BioMetals</i> , 2019, 32, 155-170.	1.8	8
10321	Synthesis and ¹³ C-Labeled O-Glycosidic Linkage Conformational Analysis of ¹³ C-Labeled Oligosaccharide Fragments of an Antifreeze Glycolipid. <i>Journal of Organic Chemistry</i> , 2019, 84, 1706-1724.	1.7	15
10322	Dehydrogenation of formic acid catalysed by M-embedded nitrogen-doped graphene (M = Fe, Ru, Os): a DFT study. <i>New Journal of Chemistry</i> , 2019, 43, 1440-1448.	1.4	15
10323	The gas phase oxidation of HCOOH by Cl and NH ₂ radicals. Proton coupled electron transfer versus hydrogen atom transfer. <i>Molecular Physics</i> , 2019, 117, 1430-1441.	0.8	6
10324	Can we rely on hybrid-DFT energies of solid-state problems with local-DFT geometries?. <i>Electronic Structure</i> , 2019, 1, 015008.	1.0	18
10325	Re-evaluating semi-empirical computer simulations in quantum chemistry. <i>Foundations of Chemistry</i> , 2019, 21, 83-95.	0.4	1
10326	Intramolecular n-type proton/hydrogen network in basic structures of vitamin B6 investigated by IRMPD spectroscopy. <i>International Journal of Mass Spectrometry</i> , 2019, 438, 148-156.	0.7	4
10327	Second hyperpolarizability of diffuse-electron compounds M-NH ₃ , M-NLi ₃ and M-NLi ₃ -M of alkaline earth metals: Effect of lithiation. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 88, 81-91.	1.3	8

#	ARTICLE	IF	CITATIONS
10328	Hydrogen Abstraction Reaction $\text{H}_2\text{Se} + \text{OH} \hat{=} \text{H}_2\text{O} + \text{SeH}$: Comparison with the Analogous Hydrogen Sulfide and Water Reactions. <i>Inorganic Chemistry</i> , 2019, 58, 2069-2079.	1.9	2
10329	Sustainable Metallocavitand for Flue Gas-Selective Sorption: A Multiscale Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 3188-3202.	1.5	5
10330	Puzzling Reaction of Imidazole with Methyl Parathion: P=S versus P=O Mechanistic Shift Dilemma in Organophosphates. <i>Chemistry - A European Journal</i> , 2019, 25, 817-822.	1.7	11
10331	The DFT/MRCI method. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1394.	6.2	99
10332	Basics of semiconducting metal oxide-based gas sensors. , 2019, , 61-165.		17
10333	Study of the reaction mechanism of oxygen to heterogeneous reduction of NO by char. <i>Fuel</i> , 2019, 236, 1213-1225.	3.4	41
10334	N-substituted dithienopyrroles as electrochemically active monomers: Synthesis, electropolymerization and spectroelectrochemistry of the polymerization products. <i>Electrochimica Acta</i> , 2019, 295, 472-483.	2.6	14
10335	In silico investigation of the coumarin-based organic semiconductors for the possible use in organic electronic devices. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3905.	0.9	10
10336	Molecular QTAIM Topology Is Sensitive to Relativistic Corrections. <i>Chemistry - A European Journal</i> , 2019, 25, 2538-2544.	1.7	9
10337	Diterpene Synthase-Catalyzed Biosynthesis of Distinct Clerodane Stereoisomers. <i>ChemBioChem</i> , 2019, 20, 111-117.	1.3	13
10338	A comparison of the structure and bonding in the donor-acceptor complexes $\text{H}_3\text{N} \hat{=} \text{BR}(\text{OH})_2$ and $\text{H}_3\text{N} \hat{=} \text{BRH}(\text{OH})$ (R = H; NH_2 , OH, and F): a computational investigation. <i>Structural Chemistry</i> , 2019, 30, 361-368.	1.0	3
10339	Synthesis and characterization of a sterically encumbered homoleptic tetraalkyliron(III) ferrate complex. <i>Polyhedron</i> , 2019, 158, 91-96.	1.0	2
10340	Computational Methods in Spectroscopy. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 1-48.	0.6	0
10341	Characterization of valeric acid using substrate of silver nanoparticles with SERS. <i>Journal of Molecular Liquids</i> , 2019, 273, 536-542.	2.3	57
10342	DNA structure change induced by guanosine radicals - A theoretical and spectroscopic study of proton radiation damage. <i>Journal of Molecular Structure</i> , 2019, 1178, 162-168.	1.8	3
10343	Electronic Modifications of Fluorescent Cytidine Analogues Control Photophysics and Fluorescent Responses to Base Stacking and Pairing. <i>Chemistry - A European Journal</i> , 2019, 25, 1249-1259.	1.7	19
10344	Spin-Crossover Assisted Spin-Switching and Rectification Action in Half-Metallic Graphitic Carbon Nitride ($\text{g-C}_4\text{N}_3$). <i>ChemPhysChem</i> , 2019, 20, 436-442.	1.0	5
10345	Shedding Light on the Basis Set Dependence of the Minnesota Functionals: Differences Between Plane Waves, Slater Functions, and Gaussians. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 557-571.	2.3	6

#	ARTICLE	IF	CITATIONS
10346	Theoretical study of the mechanism of the manganese catalase KatB. <i>Journal of Biological Inorganic Chemistry</i> , 2019, 24, 103-115.	1.1	4
10347	Performance of DFT for C ₆₀ Isomerization Energies: A Noticeable Exception to Jacob's Ladder. <i>Journal of Physical Chemistry A</i> , 2019, 123, 257-266.	1.1	19
10348	Thermochemical Properties: Enthalpy, Entropy, and Heat Capacity of C ₂ -C ₃ Fluorinated Aldehydes. Radicals and Fluorocarbon Group Additivity. <i>Journal of Physical Chemistry A</i> , 2019, 123, 650-665.	1.1	12
10349	Unraveling the concerted catalytic mechanism of the human immunodeficiency virus type 1 (HIV-1) protease: a hybrid QM/MM study. <i>Structural Chemistry</i> , 2019, 30, 409-417.	1.0	15
10350	Designing Reactions with Post-Transition-State Bifurcations: Asynchronous Nitrene Insertions into C=C Ć Ć Bonds. <i>CheM</i> , 2019, 5, 227-236.	5.8	28
10351	Ion-Ion Repulsions and Charge-Shielding Effects Dominate the Permeation Mechanism through the OmpF Porin Channel. <i>Journal of Physical Chemistry B</i> , 2019, 123, 86-94.	1.2	6
10352	The Challenging in silico Description of Carbon Monoxide Oxidation as Catalyzed by Molybdenum-Copper CO Dehydrogenase. <i>Frontiers in Chemistry</i> , 2018, 6, 630.	1.8	8
10353	Ab initio calculation for isomerization reaction kinetics of nitrobenzene isomers. <i>Chemical Physics Letters</i> , 2019, 715, 244-251.	1.2	5
10354	Assessment of Functionals for TDDFT Calculations of One- and Two-Photon Absorption Properties of Neutral and Anionic Fluorescent Proteins Chromophores. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 490-508.	2.3	27
10355	Selective chemosensor phthalocyanines for Pd ²⁺ ions; synthesis, characterization, quantum chemical calculation, photochemical and photophysical properties. <i>Journal of Molecular Structure</i> , 2019, 1180, 127-138.	1.8	26
10356	Density functional theory. , 2019, , 119-159.		7
10357	Rhodanine-3-acetic acid containing D-Ć-A push-pull chromophores: Effect of methoxy group on the performance of dye-sensitized solar cells. <i>Organic Electronics</i> , 2019, 65, 386-393.	1.4	21
10358	The Origin of the Reproduction of Different Nitrogen Uptakes in Covalent Organic Frameworks (COFs). <i>Chemistry - A European Journal</i> , 2019, 25, 2303-2312.	1.7	13
10359	Coupled cluster theory with the polarizable continuum model of solvation. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25710.	1.0	18
10360	Molecular simulation of the structure of folate and antifolates at physiological conditions. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 87, 172-184.	1.3	12
10361	Nickel(II) NHC-complexes with tridentate, dianionic ligands. <i>Journal of Organometallic Chemistry</i> , 2019, 881, 45-50.	0.8	3
10362	Hydrogen atom transfer in the radical cations of tryptophan-containing peptides AW and WA studied by mass spectrometry, infrared multiple-photon dissociation spectroscopy, and theoretical calculations. <i>European Journal of Mass Spectrometry</i> , 2019, 25, 112-121.	0.5	6
10363	The synthesis and characterization of 1-(Allyl)-3-(2-methylbenzyl)benzimidazolium chloride: FT-IR, NMR, and DFT computational investigation. <i>Journal of Molecular Structure</i> , 2019, 1178, 212-221.	1.8	25

#	ARTICLE	IF	CITATIONS
10364	The Role of Electronic Triplet States and High-Lying Singlet States in the Deactivation Mechanism of the Parent BODIPY: An ADC(2) and CASPT2 Study. <i>ChemPhotoChem</i> , 2019, 3, 727-738.	1.5	21
10365	X-ray absorption signatures of hydrogen-bond structure in water-alcohol solutions. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25802.	1.0	13
10366	Experimental and theoretical studies on the atmospheric degradation of 1, 1, 2, 2, 3, 3, 4-heptafluorocyclopentane. <i>Atmospheric Environment</i> , 2019, 196, 38-43.	1.9	12
10367	Adsorption of phenolic compounds from water by a novel ethylenediamine rosin-based resin: Interaction models and adsorption mechanisms. <i>Chemosphere</i> , 2019, 214, 821-829.	4.2	61
10368	Synthesis, spectral characterization, DFT and photosensitivity studies of 1-[[[(4-methoxy-5-oxo-5H-furo) Tj ETQq0 0 0 rgBT /Overlock 10 Optik, 2019, 178, 1163-1176.	1.4	16
10369	Density Functional Theory Study of $M_{i+1}AX_n$ Phases: A Review. <i>Critical Reviews in Solid State and Materials Sciences</i> , 2019, 44, 56-107.	6.8	46
10370	Xylarodons A and B, new hexaketides from the endophytic fungus <i>Xylaria</i> sp. SC1440. <i>Journal of Asian Natural Products Research</i> , 2019, 21, 343-350.	0.7	3
10371	Atmospheric oxidation chemistry of 1-methoxy-propyl acetate initiated by OH radicals: kinetics and mechanisms. <i>Molecular Physics</i> , 2020, 118, e1601786.	0.8	4
10372	Halogenated derivatives of methotrexate as human dihydrofolate reductase inhibitors in cancer chemotherapy. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 901-917.	2.0	12
10373	Zinc(II) and mercury(II) iodide complexes containing 2-pyridinealldoxime compound: synthesis, characterization, crystal structure determination and DFT study. <i>Journal of the Iranian Chemical Society</i> , 2020, 17, 441-451.	1.2	5
10374	Tuning of structural and magnetic properties by intriguing radical-radical interaction by double electron oxidation in U-A-U ² triplex formation. <i>Chemical Physics</i> , 2020, 528, 110527.	0.9	0
10375	Highly-efficient upconversion via direct one-photon absorption of xanthene-based chromophores. <i>Dyes and Pigments</i> , 2020, 172, 107853.	2.0	12
10376	Ga-doped phagraphene as a superior media for sensing of carbon monoxide: A detailed theoretical investigation. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 116, 113710.	1.3	29
10377	Fabrication and characterization of luminescent Pr ³⁺ doped fluorapatite nanocrystals as bioimaging contrast agents. <i>Journal of Luminescence</i> , 2020, 217, 116757.	1.5	21
10378	Mechanisms of supramolecular ordering of water-soluble derivatives of fullerenes in aqueous media. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2020, 28, 30-39.	1.0	6
10379	Novel biologically active metallophthalocyanines as promising antioxidant-antibacterial agents: Synthesis, characterization and computational properties. <i>Journal of Molecular Structure</i> , 2020, 1200, 127127.	1.8	39
10380	Adsorption of small gas molecules on transition metal (Fe, Ni and Co, Cu) doped graphene: A systematic DFT study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 116, 113768.	1.3	65
10381	Sensitive SERS detection and characterization of procaine in aqueous media by reduced gold nanoparticles. <i>Sensors and Actuators B: Chemical</i> , 2020, 304, 127057.	4.0	44

#	ARTICLE	IF	CITATIONS
10382	Ion spectroscopy of heterogeneous mixtures: IRMPD and DFT analysis of anomers and conformers of monosaccharides. <i>International Journal of Mass Spectrometry</i> , 2020, 447, 116235.	0.7	14
10383	Comparison of the yields of mono-, Di- and tri-chlorinated HAAs and THMs in chlorination and chloramination based on experimental and quantum-chemical data. <i>Water Research</i> , 2020, 169, 115100.	5.3	17
10384	Ab initio modeling and design of vanadia-based electrode materials for post-lithium batteries. <i>Journal Physics D: Applied Physics</i> , 2020, 53, 083001.	1.3	9
10385	Computational and electrochemical analysis on quinoxalines as corrosion inhibitors for mild steel in acidic medium. <i>Journal of Molecular Liquids</i> , 2020, 297, 111883.	2.3	43
10386	Thioether-linked liquid crystal dimers and trimers: The twist-bend nematic phase. <i>Journal of Molecular Structure</i> , 2020, 1199, 126913.	1.8	42
10387	Tunable fluorescent pyrene/diarylethene-based bistable [3]rotaxane. <i>Dyes and Pigments</i> , 2020, 172, 107800.	2.0	12
10388	Modeling the action of environment on proton tunneling in the adenine-thymine base pair. <i>Progress in Biophysics and Molecular Biology</i> , 2020, 150, 98-103.	1.4	8
10389	Mechanism and Inhibitor Exploration with Binuclear Mg Ketolâ€Acid Reductoisomerase: Targeting the Biosynthetic Pathway of Branchedâ€Chain Amino Acids. <i>ChemBioChem</i> , 2020, 21, 381-391.	1.3	4
10390	Novel blue-green emitting NLOphoric triphenylamine-imidazole based donor-â€acceptor compound: Solvatochromism, DFT, TD-DFT and non-linear optical studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117421.	2.0	25
10391	New small organic molecules based on thieno[2,3-b]indole for efficient bulk heterojunction organic solar cells: a computational study. <i>Molecular Physics</i> , 2020, 118, e1662956.	0.8	36
10392	Experimental and theoretical approach to the corrosion inhibition of mild steel in acid medium by a newly synthesized pyrazole carbothioamide heterocycle. <i>Journal of Molecular Structure</i> , 2020, 1199, 127051.	1.8	67
10393	Molecular properties of 5-(1H-Benzo[D]Oxa, thia, imidazole-2-yl)-2-methyl quinazolin-4-ol fluorescent brighteners: Theoretical and experimental approach. <i>Journal of Molecular Structure</i> , 2020, 1199, 126984.	1.8	5
10394	Quantum chemical calculation studies of Pd _n Si ₁₂ (n=1,2,3) clusters: effects of doping Pd atoms on the structural and electronic properties. <i>Molecular Physics</i> , 2020, 118, e1656350.	0.8	2
10395	Switching of opticalâ€resolution selectivity through the Onsager's reaction field: Chiral recognition of dl â€amino acids by hydrophilic/hydrophobic chitosans. <i>Journal of Applied Polymer Science</i> , 2020, 137, 48317.	1.3	0
10396	Theoretical study on decomposition pathways and reaction rate constants of C ₄ F ₇ N with O atom. <i>Journal Physics D: Applied Physics</i> , 2020, 53, 105202.	1.3	13
10397	Synthesis and properties of ipsilateral double substituted diphenylsulfone thermally activated delayed fluorescent materials. <i>Dyes and Pigments</i> , 2020, 174, 108028.	2.0	2
10398	Theoretical Study on Factors Influencing the Efficiency of Dâ€A Isoindigo-Based Sensitizer for Dye-Sensitized Solar Cells. <i>Journal of Electronic Materials</i> , 2020, 49, 318-332.	1.0	11
10399	The effect of molecular structure on the properties of quinoxaline-based molecules for OLED applications. <i>Dyes and Pigments</i> , 2020, 173, 108008.	2.0	34

#	ARTICLE	IF	CITATIONS
10400	From a week to less than a day: Speedup and scaling of coordinate-scaled exact exchange calculations in plane waves. <i>Computer Physics Communications</i> , 2020, 247, 106943.	3.0	5
10401	Isoxazolone Reactivity Explained by Computed Electronic Structure Analysis. <i>Chinese Journal of Chemistry</i> , 2020, 38, 163-168.	2.6	7
10402	Ether based flexible bis Schiff base fluorescent colorimetric chemosensors for selective and sensitive detection of HF ₂ ⁻ ion. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 389, 112179.	2.0	5
10403	New complexes of manganese (II) and copper (II) derived from the two new furofuran-3, 4-dione ligands: Synthesis, spectral characterization, ESR, DFT studies and evaluation of antimicrobial activity. <i>Journal of Molecular Structure</i> , 2020, 1202, 127307.	1.8	16
10404	Dynamical fluxionality, multiplicity of geometrical forms, and electronic properties of anionic, neutral, and cationic Ta _n Si ₁₂ (n = 1-3) clusters: quantum chemical calculations. <i>Molecular Physics</i> , 2020, 118, e1682209.	0.8	6
10405	Through-space Effect between the Bridging Oxygen Atoms in Diepoxybenzo[de]isothiochromene Derivatives. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 156-161.	1.2	7
10406	Supramolecular assembly of a 2D coordination polymer bearing pyridine-N-oxide-2,5-dicarboxylic acid and copper ion: X-ray crystallography and DFT calculations. <i>Journal of Molecular Structure</i> , 2020, 1202, 127243.	1.8	22
10407	Harmines derivatives: a comprehensive quantum chemical investigation of the structural, electronic (FMO, NBO, and MEP), and spectroscopic (FT-IR and UV-Vis) properties. <i>Research on Chemical Intermediates</i> , 2020, 46, 961-982.	1.3	27
10408	Tuning optoelectronic properties of triphenylamine based dyes through variation of pi-conjugated units and anchoring groups: A DFT/TD-DFT investigation. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 94, 107480.	1.3	31
10409	In silico prediction of a new lead compound targeting enolase of trypanosomatids through structure-based virtual screening and molecular dynamic studies. <i>Journal of Molecular Modeling</i> , 2020, 26, 23.	0.8	2
10410	Hydration and aggregation of a simple amino acid: The case of glycine. <i>Journal of Molecular Liquids</i> , 2020, 301, 112407.	2.3	18
10411	Synthesis of Expanded Hetero 2,6-Pyrihexaphyrins. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 736-743.	1.2	10
10412	A comprehensive study on molecular geometry, optical, HOMO-LUMO, and nonlinear properties of 1,3-diphenyl-2-propen-1-ones chalcone and its derivatives for optoelectronic applications: A computational approach. <i>Optik</i> , 2020, 204, 164172.	1.4	30
10413	Influence of Electrolyte Composition on Ultrafast Interfacial Electron Transfer in Fe-Sensitized TiO ₂ -Based Solar Cells. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1794-1811.	1.5	19
10414	Dinuclear copper(II) complexes containing oxamate and blocking ligands: crystal structure, magnetic properties, and DFT calculations. <i>New Journal of Chemistry</i> , 2020, 44, 2597-2608.	1.4	6
10415	Acceptor tuning effect on TPA-based organic efficient sensitizers for optoelectronic applications: quantum chemical investigation. <i>Structural Chemistry</i> , 2020, 31, 1029-1042.	1.0	15
10416	Designing aromatic heterocyclic superacids in terms of Brønsted and Lewis perspectives. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1923-1931.	1.3	7
10417	Mechanism and stereoselectivity of benzylic C-H hydroxylation by Ru-porphyrin: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 346-352.	1.5	8

#	ARTICLE	IF	CITATIONS
10418	Mechanism and kinetics of astrophysically relevant gas-phase stereoinversion in glutamic acid: A computational study. <i>Molecular Astrophysics</i> , 2020, 18, 100061.	1.7	7
10419	An Efficient Coupled-Perturbed Kohn-Sham Implementation of NMR Chemical Shift Computations with Local Hybrid Functionals and Gauge-Including Atomic Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 931-943.	2.3	34
10420	Reactions of a distonic peroxy radical anion influenced by SOMO-HOMO conversion: an example of anion-directed channel switching. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2130-2141.	1.3	9
10421	Rational design of a high-efficiency, multivariate metal-organic framework phosphor for white LED bulbs. <i>Chemical Science</i> , 2020, 11, 1814-1824.	3.7	43
10422	Dinuclear μ_2 -Phenoxy and μ_2 -Hydroxo Bridged Copper Complexes Exhibiting Oxidation of Phenols and Isoelectronic Compounds: Cytotoxicity and Evidences for Cellular Apoptosis. <i>ChemistrySelect</i> , 2020, 5, 463-475.	0.7	1
10423	Insight into the reaction mechanism and chemoselectivity in the cycloaddition of ynamides and isoxazoles with H_2O . <i>Catalysis Science and Technology</i> , 2020, 10, 240-251.	2.1	9
10424	Dithienothiazine dimers, trimers and polymers - novel electron-rich donors with red-shifted luminescence. <i>Materials Chemistry Frontiers</i> , 2020, 4, 621-630.	3.2	6
10425	Diversity-oriented approach to functional thiophene dyes by Suzuki coupling-lithiation one-pot sequences. <i>Organic Chemistry Frontiers</i> , 2020, 7, 329-339.	2.3	8
10426	A molecular orbital selection approach for fast calculations of specific rotation with density functional theory. <i>Chirality</i> , 2020, 32, 243-253.	1.3	3
10427	Constructing spin-adiabatic states for the modeling of spin-crossing reactions. I. A shared-orbital implementation. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26123.	1.0	3
10428	Five- and six-member bowl-shaped structures from acylphloroglucinols: an ab initio and DFT study. <i>Journal of Molecular Modeling</i> , 2020, 26, 13.	0.8	7
10429	Benchmark study of DFT and composite methods for bond dissociation energies in argon compounds. <i>Chemical Physics</i> , 2020, 531, 110676.	0.9	8
10430	Synthesis of a novel phenytoin derivative: Crystal structure, Hirshfeld surface analysis and DFT calculations. <i>Journal of Molecular Structure</i> , 2020, 1205, 127630.	1.8	56
10431	A new chromenylium-cyanine chemosensor for switch-ON near-infrared copper (II) sensing. <i>Journal of Molecular Structure</i> , 2020, 1205, 127640.	1.8	7
10432	Synthesis, crystal structure, Hirshfeld surface analysis and DFT calculations of 2-[(2,3-dimethylphenyl)amino]-N TM -[(E)-thiophen-2-ylmethylidene]benzohydrazide. <i>Journal of Molecular Structure</i> , 2020, 1205, 127654.	1.8	76
10433	On the physical-chemical nature of solvent polarizability and dipolarity. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 229, 118008.	2.0	12
10434	Redox-Associated Variation of Hückel Aromaticity from Lactam-Embedded Smallest Antiaromatic trans-Doubly N-Confused Porphyrins: Synthesis and Characterization. <i>Journal of Organic Chemistry</i> , 2020, 85, 2059-2067.	1.7	14
10435	Role of Boron in Enhancing the Catalytic Performance of Supported Platinum Catalysts for the Nonoxidative Dehydrogenation of <i>n</i> -Butane. <i>ACS Catalysis</i> , 2020, 10, 1500-1510.	5.5	21

#	ARTICLE	IF	CITATIONS
10436	Mechanism of Cobalt-Catalyzed Direct Aminocarbonylation of Unactivated Alkyl Electrophiles: Outer-Sphere Amine Substitution To Form Amide Bond. <i>ACS Catalysis</i> , 2020, 10, 1520-1527.	5.5	18
10437	Oxidative Degradation Kinetics and Mechanism of Two Biodiesel Constituents (Ethyl-2-Methyl) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Space Chemistry, 2020, 4, 142-156.	1.2	3
10438	The kinetic study of the methane oxidation reaction catalyzed by transition metal oxides RuO/RhO/PdO. <i>Molecular Simulation</i> , 2020, 46, 350-355.	0.9	0
10439	Photoelectrochemistry of Ferrites: Theoretical Predictions vs. Experimental Results. <i>Zeitschrift Fur Physikalische Chemie</i> , 2020, 234, 719-776.	1.4	24
10440	Molecular design of novel indacenodithiophene-based organic dyes for efficient dye-sensitized solar cells applications. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26147.	1.0	7
10441	Inhibitory effect of Pistacia khinjuk aerial part extract for carbon steel corrosion in sulfuric acid and hydrochloric acid solutions. <i>Chemical Papers</i> , 2020, 74, 1799-1815.	1.0	14
10442	Spirocyclic lactams and curvulinic acid derivatives from the endophytic fungus <i>Curvularia lunata</i> and their antibacterial and antifungal activities. <i>F-terap-A</i> , 2020, 141, 104466.	1.1	7
10443	Deep Red Iridium(III) Complexes Based on Pyrene-Substituted Quinoxaline Ligands for Solution-Processed Phosphorescent Organic Light-Emitting Diodes. <i>Inorganic Chemistry</i> , 2020, 59, 332-342.	1.9	24
10444	New cyanopyridine based conjugated polymers carrying auxiliary electron donors: From molecular design to blue emissive PLEDs. <i>Dyes and Pigments</i> , 2020, 174, 108046.	2.0	11
10445	Highly efficient blue-emitting of bis-cyclometalated tetravalent platinum (IV) complexes: A theoretical study. <i>Inorganica Chimica Acta</i> , 2020, 501, 119269.	1.2	4
10446	A DFT probe on the linear and nonlinear optical characteristics of some star-shaped D _{3h} acetylene-bridged rigid triazines. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4027.	0.9	4
10447	Solvation of Co ²⁺ ion in 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquid: A molecular dynamics and X-ray absorption study. <i>Journal of Molecular Liquids</i> , 2020, 299, 112120.	2.3	24
10448	Properties of monolayer black phosphorus affected by uniaxial strain. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 117, 113834.	1.3	5
10449	Synthetic and mechanistic studies in enantioselective allylic substitutions catalysed by palladium complexes of a modular class of axially chiral quinazoline-containing ligands. <i>Tetrahedron</i> , 2020, 76, 130780.	1.0	8
10450	Auxiliary hydroxy-phenanthro [9, 10-d] imidazole supported NLOphoric triphenylamine based donor-pi-acceptor compounds: Synthesis, solvatochromism and computational aspects. <i>Journal of Luminescence</i> , 2020, 219, 116902.	1.5	6
10451	Strong Collectivity of Optical Transitions in Lead Halide Perovskite Quantum Dots. <i>Plasmonics</i> , 2020, 15, 581-590.	1.8	5
10452	Importance of self-interaction-error removal in density functional calculations on water cluster anions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3789-3799.	1.3	32
10453	Layered Cathode Materials for Lithium-Ion Batteries: Review of Computational Studies on LiNi _{1-x-y} Co _x Mn _y O ₂ and LiNi _{1-x-y} Co _x Al _y O ₂ . <i>Chemistry of Materials</i> , 2020, 32, 915-952.	3.2	196

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10454	Solvatochromic Parameters of Deep Eutectic Solvents: Effect of Different Carboxylic Acids as Hydrogen Bond Donor. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 640-646.	1.0	60
10455	Dibenzofuran/Dibenzothiophene-Embedded Dithia-bis(calix)-sapphyrins. <i>Journal of Organic Chemistry</i> , 2020, 85, 2180-2189.	1.7	18
10456	Generation of molybdenum hydride species via addition of molecular hydrogen across metal-oxygen bond at monolayer oxide/metal composite interface. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 2975-2988.	3.8	10
10457	Rational Design of a Near-Infrared Fluorescence Probe for Ca ²⁺ Based on Phosphorus-Substituted Rhodamines Utilizing Photoinduced Electron Transfer. <i>Chemistry - an Asian Journal</i> , 2020, 15, 524-530.	1.7	14
10458	Kinetics of the hydrogen abstraction alkane + O ₂ → alkyl + HO ₂ reaction class: an application of the reaction class transition state theory. <i>Structural Chemistry</i> , 2020, 31, 731-746.	1.0	1
10459	On the hypergolicity of trimethyl aluminum in air. <i>Computational and Theoretical Chemistry</i> , 2020, 1173, 112668.	1.1	5
10460	Microscopic Mechanisms of N ₂ O ₅ Hydrolysis on the Surface of Water Droplets. <i>Journal of Physical Chemistry A</i> , 2020, 124, 224-228.	1.1	9
10461	Noncollinear Relativistic Two-Component X2C Calculations of Hyperfine Couplings Using Local Hybrid Functionals. Importance of the High-Density Coordinate Scaling Limit. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 314-325.	2.3	19
10462	Empirical Double-Hybrid Density Functional Theory: A "Third Way" in Between WFT and DFT. <i>Israel Journal of Chemistry</i> , 2020, 60, 787-804.	1.0	129
10463	Benchmarking Electronic Structure Methods for Accurate Fixed-Charge Electrostatic Models. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 249-258.	2.5	12
10464	Benchmark Study of Ground-State Raman Spectra in Conjugated Molecules. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 612-620.	2.3	6
10465	Tunable linear and nonlinear optical properties of chromophores containing 3,7-(di)vinylquinoxalinone core by modification of receptors moieties. <i>Optical Materials</i> , 2020, 99, 109580.	1.7	19
10466	Synthesis and investigation of BODIPYs with restricted <i>meso</i> -8-aryl rotation. <i>Journal of Porphyrins and Phthalocyanines</i> , 2020, 24, 869-877.	0.4	5
10467	Trapping of Polysulfides with Sulfur-Rich Poly Ionic Liquid Cathode Materials for Ultralong-Life Lithium-Sulfur Batteries. <i>ChemSusChem</i> , 2020, 13, 715-723.	3.6	41
10468	Computational study of [(phenanthroline) ₂ Fe ^{II} /(III)â“(terephthalate)â“Co ^{III} /II(phenanthroline) ₂] ³⁺ binuclear complex. <i>Structural Chemistry</i> , 2020, 31, 809-821.	1.0	1
10469	Analysis of Density-Functional Errors for Noncovalent Interactions between Charged Molecules. <i>Journal of Physical Chemistry A</i> , 2020, 124, 353-361.	1.1	5
10470	Light-Induced excited spin-state trapping in spin crossover model system. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26122.	1.0	2
10471	Computational Study on the Light-Induced Oxidation of Iridium-Aqua Complex to Iridium-Oxo Complex over WO ₃ (001) Surface. <i>Inorganic Chemistry</i> , 2020, 59, 415-422.	1.9	4

#	ARTICLE	IF	CITATIONS
10472	Alkyl-Group-Wrapped Unsymmetrical Squaraine Dyes for Dye-Sensitized Solar Cells: Branched Alkyl Chains Modulate the Aggregation of Dyes and Charge Recombination Processes. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 2555-2565.	4.0	31
10473	A Comprehensive Study on Self-Assembly and Gelation of C ₁₃ -Dipeptides From Design Strategies to Functionalities. <i>Biomacromolecules</i> , 2020, 21, 670-679.	2.6	13
10474	Influencing the Self-Sorting Behavior of [2.2]Paracyclophane-Based Ligands by Introducing Isostructural Binding Motifs. <i>Chemistry - A European Journal</i> , 2020, 26, 3335-3347.	1.7	12
10475	A DFT study on radical-cationic methanol clusters: Structure, bonding and H-transfer. <i>Computational and Theoretical Chemistry</i> , 2020, 1171, 112661.	1.1	0
10476	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 587-600.	2.3	69
10477	Expedition on surface adsorption of N-nitrosodiethylamine from rubber fumes on blue phosphorene sheets – a first-principles insight. <i>Molecular Physics</i> , 2020, 118, e1699184.	0.8	11
10478	Understanding the role of hydrogen bonds in destruction of DNA by screening interactions of Flutamide anticancer drug with nucleotides bases: DFT perspective, MD simulation and free energy calculation. <i>Adsorption</i> , 2020, 26, 491-508.	1.4	0
10479	Influence of orthogonal di- and trimerization leading to meso fused BODIPY on linear and NLO properties - TDDFT study and singlet-triplet energy distribution. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 389, 112284.	2.0	4
10480	Kinetics and Thermodynamics of Reactions Involving Criegee Intermediates: An Assessment of Density Functional Theory and Ab Initio Methods Through Comparison with CCSDT(Q)/CBS Data. <i>Journal of Computational Chemistry</i> , 2020, 41, 328-339.	1.5	13
10481	Density Functional Extension to Excited-State Mean-Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 164-178.	2.3	22
10482	Combining Embedded Mean-Field Theory with Linear-Scaling Density-Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 354-365.	2.3	3
10483	Visible-Light-Assisted Gasochromic Sensing of Nicotine from Cigarette Smoke by Metal-Organic Nanotube. , 2020, 2, 9-14.		15
10484	Role of chemical pressure on optical and electronic structure of Ho ₂ Ge ₂ Ti ₂ O ₇ . <i>Journal of Physics Condensed Matter</i> , 2020, 32, 115501.	0.7	5
10485	Enthalpy of formation for indazoles (indazole, 1H-indazole-3-carboxylic acid, 1H-indazole-5-carboxylic) and theoretical studies. <i>Journal of Thermal Analysis and Calorimetry</i> , 2020, 141, 819-828.	2.0	2
10486	Au ₂ Si ₂₀ : a honeycomb-shaped structure with short Au~Au single bond at the centre coordinated by twelve Si ₅ pentagons and reinforced by strong Au~Si interactions and aromaticity. <i>Molecular Physics</i> , 2020, 118, e1692152.	0.8	4
10487	The Decomposition Pathways of SF ₆ in the Presence of Organic Insulator Vapors. <i>Plasma Chemistry and Plasma Processing</i> , 2020, 40, 449-467.	1.1	9
10488	Interaction of antitubercular drug candidates with Î±1-acid glycoprotein produced in pulmonary granulomas. <i>International Journal of Biological Macromolecules</i> , 2020, 147, 1318-1327.	3.6	7
10489	Importance of the iron-sulfur component and of the siroheme modification in the resting state of sulfite reductase. <i>Journal of Inorganic Biochemistry</i> , 2020, 203, 110928.	1.5	4

#	ARTICLE	IF	CITATIONS
10490	Ligand-Mediated Regioselective Rhodium-Catalyzed Benzotriazole-Allene Coupling: Mechanistic Exploration and Quantum Chemical Analysis. <i>Chemistry - A European Journal</i> , 2020, 26, 2342-2348.	1.7	16
10491	New N-ribosides and N-mannosides of rhodanine derivatives with anticancer activity on leukemia cell line: Design, synthesis, DFT and molecular modelling studies. <i>Carbohydrate Research</i> , 2020, 487, 107894.	1.1	26
10492	Is It Conjugated or Not? The Theoretical and Experimental Electron Density Map of Bonding in p-CH ₃ CH ₂ COC ₆ H ₄ -C ₆ H ₄ -C ₆ H ₄ COCH ₃ CH ₂ . <i>Molecules</i> , 2020, 25, 4388.	1.7	1
10493	Chemical kinetics study of 1,3-butadiene; implications for combustion modeling and simulation. <i>Combustion and Flame</i> , 2020, 221, 241-255.	2.8	10
10494	Unraveling the energetic significance of chemical events in enzyme catalysis via machine-learning based regression approach. <i>Communications Chemistry</i> , 2020, 3, .	2.0	16
10495	1,2,4-Triazolato paddlewheel dibismuth complexes with very short Bi(ii)-Bi(ii) bonds: bismuth(iii) oxidation of 1,2,4-triazolato anions into neutral N-1,2,4-triazolyl radicals. <i>Dalton Transactions</i> , 2020, 49, 15190-15194.	1.6	1
10496	QSAR and docking molecular models to predict anti-cancer activity on a series of azacalix [2] arene [2] pyrimidine derivatives as anticancer agents. <i>Materials Today: Proceedings</i> , 2020, , .	0.9	2
10497	QSAR modeling, molecular docking studies and ADMET prediction on a series of phenylaminopyrimidine-(thio) urea derivatives as CK2 inhibitors. <i>Materials Today: Proceedings</i> , 2022, 51, 1851-1862.	0.9	4
10498	On the Correlation Potential in Frozen-Density Embedding Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6880-6885.	2.3	15
10499	Hole Polaron Transport in Bismuth Vanadate BiVO ₄ from Hybrid Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23038-23044.	1.5	20
10500	Synthesis, Structure, Dynamics, and Enantioface-Selective η^3 -Benzyl Coordination in the Chiral Rhodium Complexes Rh(diphos*)(η^3 -CH ₂ Ph). <i>Organometallics</i> , 2020, 39, 3802-3816.	1.1	3
10501	Theoretical study on functionalized acrylonitrile compounds with a large second-order nonlinear optical response. <i>New Journal of Chemistry</i> , 2020, 44, 19623-19629.	1.4	7
10502	Quantum Chemical Calculation and DFT Study of Sitagliptin: Insight from Computational Evaluation and Docking Approach. <i>Journal of Nepal Physical Society</i> , 2020, 6, 73-83.	0.1	1
10504	Trifunctional epoxy resin as anticorrosive material for carbon steel in 1 M HCl: Experimental and computational studies. <i>Surfaces and Interfaces</i> , 2020, 21, 100707.	1.5	13
10505	CRAHCN-O: A Consistent Reduced Atmospheric Hybrid Chemical Network Oxygen Extension for Hydrogen Cyanide and Formaldehyde Chemistry in CO ₂ , N ₂ , H ₂ O, CH ₄ , and H ₂ -Dominated Atmospheres. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8594-8606.	1.1	4
10506	Evaluation of Single-Reference DFT-Based Approaches for the Calculation of Spectroscopic Signatures of Excited States Involved in Singlet Fission. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8446-8460.	1.1	10
10507	Theoretical study on the catalytic mechanism of human deoxyhypusine hydroxylase. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22736-22745.	1.3	6
10508	Half-sandwich complexes of osmium containing guanidine-derived ligands. <i>Dalton Transactions</i> , 2020, 49, 13601-13617.	1.6	10

#	ARTICLE	IF	CITATIONS
10509	Synthesis and properties of 6,7-dihydroxybenzopyrylium perchlorate halogen derivatives: X-ray, spectroscopic and theoretical studies. <i>Tetrahedron</i> , 2020, 76, 131514.	1.0	10
10510	Tunable from Blue to Red Emissive Composites and Solids of Silver Diphosphane Systems with Higher Quantum Yields than the Diphosphane Ligands. <i>Inorganic Chemistry</i> , 2020, 59, 14447-14456.	1.9	9
10511	Method for the accurate prediction of electron transfer potentials using an effective absolute potential. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25833-25840.	1.3	15
10512	A theoretical investigation on conformers of imidazolium salts. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	0
10513	Design and synthesis of coumarin-triazole hybrids: biocompatible anti-diabetic agents, in silico molecular docking and ADME screening. <i>Heliyon</i> , 2020, 6, e05290.	1.4	19
10514	An extensive investigation of structural, electronic, thermoelectric and optical properties of bi-based half-Huesler alloys by first principles calculations. <i>Materials Today Communications</i> , 2020, 25, 101647.	0.9	9
10515	First-Principles Modeling of Oxygen-Deficient Anatase TiO ₂ Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23637-23647.	1.5	13
10516	Calculation of magnetic properties with density functional approximations including rung 3.5 ingredients. <i>Journal of Chemical Physics</i> , 2020, 153, 164101.	1.2	1
10517	Synthesis, spectral analysis, molecular docking and DFT studies of 3-(2, 6-dichlorophenyl)-acrylamide and its dimer through QTAIM approach. <i>Heliyon</i> , 2020, 6, e05016.	1.4	3
10518	Speciation, thermodynamics and structure of Np(^v) oxalate complexes in aqueous solution. <i>Dalton Transactions</i> , 2020, 49, 13359-13371.	1.6	4
10519	NBO/NRT Two-State Theory of Bond-Shift Spectral Excitation. <i>Molecules</i> , 2020, 25, 4052.	1.7	9
10520	Protein Matrix Control of Reaction Center Excitation in Photosystem II. <i>Journal of the American Chemical Society</i> , 2020, 142, 18174-18190.	6.6	46
10521	Boron extraction from lithium-rich brine using mixed alcohols. <i>Hydrometallurgy</i> , 2020, 197, 105477.	1.8	15
10522	Transferability of self-energy correction in tight-binding basis constructed from first principles. <i>Journal of Chemical Physics</i> , 2020, 153, 144103.	1.2	2
10523	Five-coordinate transition metal complexes and the value of $\langle i \rangle_{i=5}$: observations and caveats. <i>Dalton Transactions</i> , 2020, 49, 14798-14806.	1.6	59
10524	Detection and Characterization of Mononuclear Pd(II) Complexes Supported by N2S2 and N4 Tetradentate Ligands. <i>Inorganic Chemistry</i> , 2020, 59, 15659-15669.	1.9	15
10525	Surface-Doped Quasi-2D Chiral Organic Single Crystals for Chiroptical Sensing. <i>ACS Nano</i> , 2020, 14, 14146-14156.	7.3	33
10526	Dimethyl and ethyl methyl ether adsorption studies on $\hat{1}^2$ -antimonene nanosheets â€“ a first-principles study. <i>Molecular Simulation</i> , 2020, 46, 1354-1361.	0.9	17

#	ARTICLE	IF	CITATIONS
10527	Stabilizing Perovskite Solar Cells to IEC61215:2016 Standards with over 9,000-h Operational Tracking. <i>Joule</i> , 2020, 4, 2646-2660.	11.7	218
10528	Density Functional Theory Investigation of As(III) S-Adenosylmethionine Methyltransferase. <i>ACS Omega</i> , 2020, 5, 21000-21006.	1.6	0
10529	The Effects of the Metal Ion Substitution into the Active Site of Metalloenzymes: A Theoretical Insight on Some Selected Cases. <i>Catalysts</i> , 2020, 10, 1038.	1.6	34
10530	Luminescent organic materials based on donor-acceptor-donor compounds containing carbazole donors and acceptors of varying strength: Spectroscopy, redox properties and application in organic light emitting diodes. <i>Optical Materials</i> , 2020, 108, 110428.	1.7	2
10531	Time-Resolved Vibrational Analysis of Excited State Ab Initio Molecular Dynamics to Understand Photorelaxation: The Case of the Pyranine Photoacid in Aqueous Solution. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6007-6013.	2.3	23
10532	Unveiling the Mechanism, Origin of Stereoselectivity, and Ligand-Dependent Reactivity in the Pd(II)-Catalyzed Unbiased Methylene C(sp ³) ³ â€”H Alkenylationâ€”Aza-Wacker Cyclization Reaction. <i>Journal of Organic Chemistry</i> , 2020, 85, 13191-13203.	1.7	7
10533	Nuclear Spinâ€”Spin Couplings: Efficient Evaluation of Exact Exchange and Extension to Local Hybrid Functionals. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8529-8539.	1.1	17
10534	Determination of thermodynamic functions and structural parameters of NpO ₂ ⁺ lactate complexes. <i>New Journal of Chemistry</i> , 2020, 44, 17033-17046.	1.4	3
10535	Theoretical determination of two-photon absorption in biologically relevant pterin derivatives. <i>Photochemical and Photobiological Sciences</i> , 2020, 19, 1538-1547.	1.6	6
10536	Phase stability and fast ion transport in P2-type layered Na ₂ X ₂ TeO ₆ (X = Mg, Zn) solid electrolytes for sodium batteries. <i>Journal of Materials Chemistry A</i> , 2020, 8, 22816-22827.	5.2	20
10537	Computational study of organic small molecules based on imidazolinone for photovoltaic applications. <i>Energy Sources, Part A: Recovery, Utilization and Environmental Effects</i> , 0, , 1-12.	1.2	7
10538	Unravelling the impact of thiophene auxiliary in new porphyrin sensitizers for high solar energy conversion. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 392, 112408.	2.0	22
10539	The role of noncovalent interactions in olefin polymerization catalysis: a further look to the fluorinated ligand effect. <i>Molecular Catalysis</i> , 2020, 494, 111118.	1.0	6
10540	Unmasking Static Correlation Error in Hybrid Kohnâ€”Sham Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5432-5440.	2.3	25
10541	The combination of halogen and hydrogen bonding: a versatile tool in coordination chemistry. <i>CrystEngComm</i> , 2020, 22, 6010-6018.	1.3	2
10542	Holeâ€”hole Tammâ€”Dancoff-approximated density functional theory: A highly efficient electronic structure method incorporating dynamic and static correlation. <i>Journal of Chemical Physics</i> , 2020, 153, 024110.	1.2	34
10543	Crystal fields of lithium rare-earth tetrafluorides and multiplet splitting of the $3d^1$ rare-earth ions. <i>Physical Review B</i> , 2020, 102, .	1.1	5
10544	Using Photoionization Efficiency Spectroscopy and Density Functional Theory to Investigate Charge Transfer Interactions in AuCe ₃ O _n Clusters. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5812-5823.	1.1	6

#	ARTICLE	IF	CITATIONS
10545	Molecular modelling of mebendazole polymorphs as a potential colchicine binding site inhibitor. <i>New Journal of Chemistry</i> , 2020, 44, 13990-13996.	1.4	54
10546	Effects of adding cyanovinyl moiety on the photovoltaic DSSCs phosphonic acid based cells. <i>Journal of Computational Electronics</i> , 2020, 19, 1629-1644.	1.3	8
10547	Investigation of the role of terminal ligands in magnetic relaxation in a series of dinuclear dysprosium complexes. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 3352-3363.	3.0	20
10548	Tube-shaped molecular structures built from acylphloroglucinols: an ab initio and DFT study. <i>Molecular Physics</i> , 2020, 118, e1784477.	0.8	1
10549	Time-Dependent Density Functional Theory Investigation of the UV-Vis Spectra of Organonitrogen Chromophores in Brown Carbon. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 311-320.	1.2	15
10550	Two-step reaction mechanism reveals new antioxidant capability of cysteine disulfides against hydroxyl radical attack. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 18216-18223.	3.3	17
10551	Insights into C=O insertion in a carbene/alkyne metathesis cascade reaction catalyzed by Rh ₂ (OAc) ₄ : a DFT study. <i>Catalysis Science and Technology</i> , 2020, 10, 5513-5524.	2.1	2
10552	First-principles calculations on high-temperature desorption loss from iridium. <i>Computational Materials Science</i> , 2020, 184, 109897.	1.4	0
10553	Temperature dependence of rate coefficients for the gas phase reaction of OH with 3-chloropropene. A theoretical and experimental study. <i>Chemical Physics Letters</i> , 2020, 755, 137757.	1.2	3
10554	N-donor stabilized complexes of nickel(II) diphenyldithiophosphates: single-crystal X-ray, HSA and computational analysis. <i>Transition Metal Chemistry</i> , 2020, 45, 531-544.	0.7	1
10555	A New Mixing of Nonlocal Exchange and Nonlocal Correlation with Multiconfiguration Pair-Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10158-10163.	2.1	21
10556	Towards a Holomorphic Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7400-7412.	2.3	5
10557	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7413-7430.	2.3	12
10558	Synthesis and structures of divalent Co, Ni, Zn and Cd complexes of mixed dichalcogen and dipnictogen ligands with corrosion inhibition properties: experimental and computational studies. <i>RSC Advances</i> , 2020, 10, 41967-41982.	1.7	25
10559	Tailored quinones support high-turnover Pd catalysts for oxidative C-H arylation with O ₂ . <i>Science</i> , 2020, 370, 1454-1460.	6.0	42
10560	Stercobilin and Urobilin in Aqueous Media: Existence of Specific H-Aggregates and Nonspecific Higher Aggregates at Different Concentrations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10053-10065.	1.1	9
10561	Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26838-26851.	1.3	9
10562	Modulating Effect of Ligand Charge on the Electronic Properties of 2Ni ²⁺ S Structures and Implications for Biological 2M ²⁺ S Sites. <i>Inorganic Chemistry</i> , 2020, 59, 17234-17243.	1.9	0

#	ARTICLE	IF	CITATIONS
10563	Electronic Excitations in Copper Oxides: Time-Dependent Density Functional Theory Calculations with a Self-Consistent Hybrid Kernel. <i>Journal of Physical Chemistry C</i> , 2020, 124, 24995-25003.	1.5	10
10564	Reaction mechanism and product branching ratios of OH+C ₂ H ₃ F reaction: A theoretical study. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 203-209.	0.6	1
10565	Fast Nonadiabatic Molecular Dynamics via Spin-Flip Time-Dependent Density-Functional Tight-Binding Approach: Application to Nonradiative Relaxation of Tetraphenylethylene with Locked Aromatic Rings. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7299-7313.	2.3	10
10566	Byproducts formed During Thiol+Acrylate Reactions Promoted by Nucleophilic Aprotic Amines: Persistent or Reactive?. <i>ChemPlusChem</i> , 2020, 85, 2466-2474.	1.3	0
10567	Theoretical Insight on the Biosensing Applications of 2D Materials. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11098-11122.	1.2	25
10568	Photochemistry of 1,5-Cyclooctadiene Platinum Complexes for Photoassisted Chemical Vapor Deposition. <i>Organometallics</i> , 2020, 39, 4565-4574.	1.1	2
10569	Nonadiabatic Dynamics Simulation of the Wavelength-Dependent Photochemistry of Azobenzene Excited to the nπ* and ππ* Excited States. <i>Journal of the American Chemical Society</i> , 2020, 142, 20680-20690.	6.6	46
10570	Theoretical study of organic sensitizers based on 2, 6-diphenyl-4H-pyranilidene/1, 3, 4-oxadiazole for dye-sensitized solar cells. <i>Journal of Molecular Modeling</i> , 2020, 26, 346.	0.8	10
10571	Computational Studies on the Mechanism and Origin of the Different Regioselectivities of Manganese Porphyrin-Catalyzed C-H Bond Hydroxylation and Amidation of Equilenin Acetate. <i>Journal of Organic Chemistry</i> , 2020, 85, 14879-14889.	1.7	17
10572	2-Pyridone-stabilized iridium silylene/silyl complexes: structure and QTAIM analysis. <i>Dalton Transactions</i> , 2020, 49, 17665-17673.	1.6	7
10573	The effect of N-heterocyclic carbene units on the absorption spectra of Fe(<i>η</i> ² -C ₂ H ₄) complexes: a challenge for theory. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27605-27616.	1.3	8
10574	Interplay between Structure and Mechanism in Reductive Dissociative Electron Transfers to Î±,Î²-â€œEpoxyketones. <i>ChemPlusChem</i> , 2020, 85, 2387-2396.	1.3	1
10575	Coassembly of C ₁₃ -Dipeptides: Gelations from Solutions and Precipitations. <i>Biomacromolecules</i> , 2020, 21, 5256-5268.	2.6	3
10576	Functionalization of Polyethyleneimine with Hollow Cyclotrimeratrylene and Its Subsequent Supramolecular Interaction with Doxorubicin. <i>Molecules</i> , 2020, 25, 5455.	1.7	6
10577	Linear and non-linear optical characteristics of some 1,3,5-triazines influenced by prototropic tautomerism: A DFT study. <i>Optical Materials</i> , 2020, 109, 110365.	1.7	2
10578	Theoretical Design of Dithienopicenocarbazole-Based Molecules by Molecular Engineering of Terminal Units Toward Promising Non-fullerene Acceptors. <i>Frontiers in Chemistry</i> , 2020, 8, 580252.	1.8	7
10579	SCC-DFTB Parameters for Fe-C Interactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9674-9682.	1.1	3
10580	Effects of perturbation order and basis set on alchemical predictions. <i>Journal of Chemical Physics</i> , 2020, 153, 144118.	1.2	14

#	ARTICLE	IF	CITATIONS
10581	Localized Bond Orbital Analysis of the Bonds of O ₂ . Journal of Physical Chemistry A, 2020, 124, 9771-9776.	1.1	3
10582	The Fermi [∞] wdin self-interaction correction for ionization energies of organic molecules. Journal of Chemical Physics, 2020, 153, 184303.	1.2	12
10583	Putative reaction mechanism of nitrogenase after dissociation of a sulfide ligand. Journal of Catalysis, 2020, 391, 247-259.	3.1	19
10584	Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene. Journal of Physical Chemistry A, 2020, 124, 9729-9737.	1.1	4
10585	First-principles investigation of the structure and electronic properties of graphene toward Li adsorption. Molecular Simulation, 2020, 46, 1522-1529.	0.9	5
10586	The preferred conformation of the tetrafluoro-1,3-dithietane [∞] isopropylamine complex as revealed by rotational spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 28339-28344.	1.3	2
10587	Removing artifacts in polarizable embedding calculations of one- and two-photon absorption spectra of fluorescent proteins. Journal of Chemical Physics, 2020, 153, 215102.	1.2	5
10588	Catalytic Mechanism of Non-Target DNA Cleavage in CRISPR-Cas9 Revealed by <i>Ab Initio</i> Molecular Dynamics. ACS Catalysis, 2020, 10, 13596-13605.	5.5	63
10589	Can Donor Ligands Make Pd(OAc) ₂ a Stronger Oxidant? Access to Elusive Palladium(II) Reduction Potentials and Effects of Ancillary Ligands via Palladium(II)/Hydroquinone Redox Equilibria. Journal of the American Chemical Society, 2020, 142, 19678-19688.	6.6	25
10590	Synthesis and electronic properties of pyridine end-capped cyclopentadithiophene-vinylene oligomers. RSC Advances, 2020, 10, 41264-41271.	1.7	4
10591	Catalytic Reduction of Oxygen by a Copper Thiosemicarbazone Complex. European Journal of Inorganic Chemistry, 2020, 2020, 4549-4555.	1.0	7
10592	Effects of electrostatic drag on the velocity of hydrogen migration [∞] pre- and post-transition state enthalpy/entropy compensation. Physical Chemistry Chemical Physics, 2020, 22, 26955-26960.	1.3	5
10593	Revealing the Inhibition Mechanism of RNA-Dependent RNA Polymerase (RdRp) of SARS-CoV-2 by Remdesivir and Nucleotide Analogues: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2020, 124, 10641-10652.	1.2	33
10594	Crystal Structure and Mechanistic Molecular Modeling Studies of Mycobacterium tuberculosis Diterpene Cyclase Rv3377c. Biochemistry, 2020, 59, 4507-4515.	1.2	6
10595	Approximately Self-Consistent Ensemble Density Functional Theory: Toward Inclusion of All Correlations. Journal of Physical Chemistry Letters, 2020, 11, 9907-9912.	2.1	10
10596	Assessing the effect of regularization on the molecular properties predicted by SCAN and self-interaction corrected SCAN meta-GGA. Physical Chemistry Chemical Physics, 2020, 22, 18060-18070.	1.3	6
10597	Application of XDM to ionic solids: The importance of dispersion for bulk moduli and crystal geometries. Journal of Chemical Physics, 2020, 153, 054121.	1.2	11
10598	A Sterically Hindered Derivative of 2,1,3-Benzotelluradiazole: A Way to the First Structurally Characterised Monomeric Tellurium [∞] Nitrogen Radical Anion. Chemistry - A European Journal, 2020, 26, 14688-14699.	1.7	11

#	ARTICLE	IF	CITATIONS
10599	Four-component relativistic computational NMR study of ferrous, cobalt and nickel bisglycinates. <i>Mendeleev Communications</i> , 2020, 30, 476-478.	0.6	3
10600	Design, synthesis, and fungicidal evaluation of novel oxysterol binding protein inhibitors for combatting resistance associated with oxathiapiprolin. <i>Pesticide Biochemistry and Physiology</i> , 2020, 169, 104673.	1.6	10
10601	Lewis Ambiphilicity of 1,2,5-Chalcogenadiazoles for Crystal Engineering: Complexes with Crown Ethers. <i>Crystal Growth and Design</i> , 2020, 20, 5868-5879.	1.4	10
10602	Electronic Effect on Bimetallic Catalysts: Cleavage of Phosphodiester Mediated by Fe(III)â€Zn(II) Purple Acid Phosphatase Mimics. <i>Inorganic Chemistry</i> , 2020, 59, 12065-12074.	1.9	10
10603	Effect of the Heteroaromatic Antenna on the Binding of Chiral Eu(III) Complexes to Bovine Serum Albumin. <i>Inorganic Chemistry</i> , 2020, 59, 12564-12577.	1.9	11
10604	Machine Learning for Absorption Cross Sections. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7199-7210.	1.1	50
10605	Ab Initio Molecular Dynamics Simulations of Solvated Electrons in Ammonia Clusters. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7205-7216.	1.2	7
10606	Why Do We Use the Materials and Operating Conditions We Use for Heterogeneous (Photo)Electrochemical Water Splitting?. <i>ACS Catalysis</i> , 2020, 10, 11177-11234.	5.5	89
10607	Kinetics of hydrogen abstraction from CH ₃ SH by OH radicals: An ab initio RRKM-based master equation study. <i>Atmospheric Environment</i> , 2020, 242, 117833.	1.9	12
10608	Variation of the Fine-Structure Constant in Model Systems for Singlet Fission. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6682-6687.	1.1	1
10609	Electrochemical and Theoretical Study of Corrosion Inhibition on Carbon Steel in 1M HCl Medium by 1,10-Bis(4-Amino-3-Methyl-1,2,4-Triazole-5-Thioyl)Decane. <i>Journal of Failure Analysis and Prevention</i> , 2020, 20, 1673-1683.	0.5	11
10610	Nanoscale oligopeptide adsorption behaviour on chlorite as revealed by scanning probe microscopy and density functional simulations. <i>Applied Clay Science</i> , 2020, 197, 105777.	2.6	5
10611	<i>Ab Initio</i> Nonadiabatic Molecular Dynamics with Holeâ€Hole Tammâ€Dancoff Approximated Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5499-5511.	2.3	27
10612	Synthesis of 2,3-disubstituted indoles <i>via</i> a tandem reaction. <i>Organic Chemistry Frontiers</i> , 2020, 7, 2689-2695.	2.3	8
10613	Kinetic study of the CN radical reaction with 2â€methylfuran. <i>International Journal of Chemical Kinetics</i> , 2020, 52, 838-851.	1.0	1
10614	The synergistic inhibitory effect and density functional theory study of 2,2â€[[[(Methyl-1H-benzotriazol-1-yl)methyl]imino]bisethanol and potassium oleate on copper in H ₂ O ₂ based alkaline slurries. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 603, 125275.	2.3	25
10615	Structural or population dynamics: what is revealed by the time-resolved photoelectron spectroscopy of 1,3-cyclohexadiene? A study with an ensemble density functional theory method. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 17567-17573.	1.3	9
10616	Energetic Triazoloâ€Triazoloâ€Furazanoâ€Pyrazines: A Promising Fused Tetracycle Building Block with Diversified Functionalities and Properties. <i>ChemistrySelect</i> , 2020, 5, 8557-8561.	0.7	8

#	ARTICLE	IF	CITATIONS
10617	Corrosion Protection of Mild Steel by a New Phosphonated Pyridines Inhibitor System in HCl Solution. <i>Advanced Engineering Forum</i> , 0, 36, 59-75.	0.3	11
10618	Metal-free Photocatalytic Aerobic Oxidative Cleavage of C-C Bonds in 1,2-Diols. <i>ChemSusChem</i> , 2020, 13, 5248-5255.	3.6	11
10619	Role of molecule-electrode coupling strength in inducing inelastic transmission spectra of Hf@C28. <i>Chemical Physics</i> , 2020, 539, 110930.	0.9	1
10620	Evaluation of the possibility of binary synthesis of VX by theoretical calculation. <i>Chemical Physics Letters</i> , 2020, 756, 137808.	1.2	1
10621	Experimental and theoretical insight into the extraction mechanism, kinetics, thermodynamics, complexation and radiolytic stability of novel calix crown ether in ionic liquid with Sr ²⁺ . <i>Journal of Molecular Liquids</i> , 2020, 316, 113864.	2.3	12
10622	Rationale Strategy to Tune the Optical Properties of Gold Catenane Nanoclusters by Doping with Silver Atoms. <i>Journal of Physical Chemistry C</i> , 2020, 124, 19368-19374.	1.5	7
10623	An Effective Approach to Obtain Near-Infrared Emission from Binuclear Platinum(II) Complexes Involving Thiophenpyridine-Isoquinoline Bridging Ligand in Solution-Processed OLEDs. <i>Chemistry - an Asian Journal</i> , 2020, 15, 3003-3012.	1.7	3
10624	Benzyl alcohol and 2-methyldecalin vapor adsorption studies on Î²-bismuthene sheets - A DFT outlook. <i>Chemical Physics Letters</i> , 2020, 755, 137819.	1.2	19
10625	Theoretical Insight into the Reaction Mechanism and Kinetics for the Criegee Intermediate of anti-PhCHO with SO ₂ . <i>Molecules</i> , 2020, 25, 3041.	1.7	2
10626	Electronic Structure of Neutral and Anionic Iron-Nitrosyl Corrole. A Multiconfigurational and Density Matrix Renormalization Group Investigation. <i>Inorganic Chemistry</i> , 2020, 59, 11493-11502.	1.9	16
10627	Generation of empirical pseudopotentials for transport applications and their application to group IV materials. <i>Journal of Applied Physics</i> , 2020, 128, .	1.1	6
10628	Fine-Tuning the Physicochemical and Electroluminescence Properties of Multiply-Substituted Bipolar Carbazoles by Functional Group Juggling. <i>ChemPhotoChem</i> , 2020, 4, 5364-5375.	1.5	2
10629	New route for synthesis of 2-(2,2-dimethoxyethyl)-1,2,3,4,5,6-hexahydro-1,5-methanoazocino[4,3-b]indole and DFT investigation. <i>Heliyon</i> , 2020, 6, e04105.	1.4	8
10630	Interaction properties of phenol and styrene from plastic fumes on Î²-Arsenene sheets: A first-principles study. <i>Physica B: Condensed Matter</i> , 2020, 597, 412405.	1.3	14
10631	An Unprecedented Ring-Contraction Mechanism in Cobalamin-Dependent Radical <i>S</i> -Adenosylmethionine Enzymes. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6812-6818.	2.1	8
10632	A first-principle perspective on electronic nematicity in FeSe. <i>Npj Quantum Materials</i> , 2020, 5, .	1.8	15
10633	An <i>ab initio</i> multireference study of reductive eliminations from organoferrates(<i>iii</i>) in the gas-phase: it is all about the spin state. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 17677-17686.	1.3	2
10634	Experimental and theoretical investigations on electronic structure of 5-(hydroxymethyl)-2-furaldehyde: An antisickling agent identified from <i>terminalia bellirica</i> . <i>Chemical Data Collections</i> , 2020, 29, 100498.	1.1	13

#	ARTICLE	IF	CITATIONS
10635	Theoretical study of the geometric and electronic characterization of carbendazim-based drug (Nocodazole). <i>Heliyon</i> , 2020, 6, e04055.	1.4	8
10636	Unprecedented stability enhancement of multiply charged anions through decoration with negative electron affinity noble gases. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13368-13372.	1.3	12
10637	Energy of Intramolecular Interactions and Structure of Metallophosphate Polycomplexes with Water Molecules and Nitrogen-Containing Compounds. <i>Russian Journal of Physical Chemistry B</i> , 2020, 14, 516-521.	0.2	2
10638	Using van der Waals heterostructures based on two-dimensional $\text{InSe} \times \text{X}_2$ (X = Mo, W) as promising photocatalysts for hydrogen production. <i>Journal of Materials Chemistry C</i> , 2020, 8, 12509-12515.	2.7	27
10639	Photophysics and ultrafast processes in rhenium(scpi) diimine dicarbonyls. <i>Dalton Transactions</i> , 2020, 49, 11565-11576.	1.6	12
10640	Quasi-relativistic study of nuclear electric quadrupole coupling constants in chiral molecules containing heavy elements. <i>Molecular Physics</i> , 2020, 118, e1797199.	0.8	2
10641	In the Iron Tricarbonyl Mediated Electrocyclic Ring Opening of 3-Heterocyclobutenes "Does Iron or Heteroatom Decide the Pathway?". <i>Russian Journal of Inorganic Chemistry</i> , 2020, 65, 1025-1031.	0.3	0
10642	Theoretical Study of the Si/C Mixed Benzenes and Their Major Valence Isomers. <i>Organometallics</i> , 2020, 39, 3041-3049.	1.1	4
10643	Thermodynamic and thermoelastic properties of wurtzite-ZnS by density functional theory. <i>American Mineralogist</i> , 2020, 105, 1212-1222.	0.9	7
10644	Dioxygen Binding to all 3d, 4d, and 5d Transition Metals from Coupled Cluster Theory. <i>ChemPhysChem</i> , 2020, 21, 2173-2186.	1.0	2
10645	Infrared and Raman spectroscopic features of clinoclone $\text{Mg}_6\text{Si}_4\text{O}_{10}(\text{OH})_8$: A density functional theory contribution. <i>Applied Clay Science</i> , 2020, 197, 105779.	2.6	13
10646	A Computational and Modeling Study of the Reaction Mechanism of <i>Staphylococcus aureus</i> Monoglycosyltransferase Reveals New Insights on the GT51 Family of Enzymes. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5513-5528.	2.5	3
10647	What Most Affects the Accuracy of ^{125}Te NMR Chemical Shift Calculations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6714-6725.	1.1	11
10648	Synthesis, photophysical and electrochemical properties of novel and highly fluorescent difluoroboron flavanone β -diketonate complexes. <i>New Journal of Chemistry</i> , 2020, 44, 14615-14631.	1.4	4
10649	Photophysical, kinetic and thermodynamic study of one-component Type II thioxanthone acetic acid photoinitiators. <i>European Polymer Journal</i> , 2020, 136, 109909.	2.6	19
10650	Synthesis, single crystal X-ray, DFT and HSA of N-donor stabilized complexes of cobalt(II) diphenyldithiophosphate: An experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2020, 1207, 127835.	1.8	7
10651	Enhanced Sulfur Dioxide Adsorption in UiO-66 Through Crystal Engineering and Chalcogen Bonding. <i>Crystal Growth and Design</i> , 2020, 20, 6139-6146.	1.4	18
10652	Improved Oxidative C-C Bond Formation Reactivity of High-Valent Pd Complexes Supported by a Pseudo-Tridentate Ligand. <i>Inorganic Chemistry</i> , 2020, 59, 11782-11792.	1.9	11

#	ARTICLE	IF	CITATIONS
10653	Conceptualization and Synthesis of the First Inositol (Decahydroxydecalin, DHD): In ⁺ Binding to β -Amyloid Protein. <i>Chemistry - A European Journal</i> , 2020, 26, 17005-17010.	1.7	2
10654	Revisiting immiscibility through DFT chemical descriptors. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	1
10655	Mixed ligand copper(II) chelates derived from an O, N, S- donor tridentate thiosemicarbazone: Synthesis, spectral aspects, FMO, and NBO analysis. <i>Polyhedron</i> , 2020, 189, 114736.	1.0	44
10656	Exploring the Conformational Landscape of Bioactive Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6575-6585.	2.3	17
10657	Basis Set Extrapolations for Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5712-5722.	2.3	13
10658	Elastic electron scattering by tetramethylmethane, tetramethylsilane, and tetramethylgermane. <i>Physical Review A</i> , 2020, 102, .	1.0	3
10659	The influence of the structural variations in the β -bridge of D- β -A organic dyes on the efficiency of dye-sensitized solar cells (DSSCs): A DFT computational study. , 2020, , .		1
10660	Sensing mechanism elucidation of a chemosensor based on a $\text{metal}^{\text{organic}}$ framework selective to explosive aromatic compounds. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26404.	1.0	14
10661	Benchmark study of density functionals for the insertions of olefin and polar monomers catalyzed by β -diimine palladium complexes. <i>Computational and Theoretical Chemistry</i> , 2020, 1187, 112942.	1.1	3
10662	Novel green phosphorene sheets to detect tear gas molecules - A DFT insight. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107706.	1.3	23
10663	Cation Radicals of Hachimoji Nucleobases. Canonical Purine and Noncanonical Pyrimidine Forms Generated in the Gas Phase and Characterized by UV-Vis Photodissociation Action Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7101-7112.	1.1	11
10664	Theoretical investigation of new organic materials for applications in organic solar cells. , 2020, , .		0
10665	Eco-friendly sodium gluconate and trisodium citrate inhibitors for low carbon steel in simulated cooling water system: Theoretical study and molecular dynamic simulations. <i>Journal of Molecular Liquids</i> , 2020, 319, 114108.	2.3	46
10666	The Non-innocent Role of Spin Traps in Monitoring Radical Formation in Copper-Catalyzed Reactions. <i>Applied Magnetic Resonance</i> , 2020, 51, 1529-1542.	0.6	3
10667	Profiling astrophysically relevant MgC ₄ H chains. An attempt to aid astronomical observations. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 498, 4316-4326.	1.6	7
10668	Structural and Energetic Features of Group 13 Element Tris(pentafluorophenyl) Complexes with Diethyl Ether. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 4442-4449.	1.0	14
10669	High energy density materials based on fluorinated bridged trinitromethyl azo triazole derivatives: a quantum chemical study of thermodynamic and energetic properties. <i>SN Applied Sciences</i> , 2020, 2, 1.	1.5	0
10670	Low band gap donor-acceptor-donor compounds containing carbazole and naphthalene diimide units: Synthesis, electropolymerization and spectroelectrochemical behaviour. <i>Electrochimica Acta</i> , 2020, 358, 136922.	2.6	16

#	ARTICLE	IF	CITATIONS
10671	Study of three new halogenated oxoquinolinecarbohydrazide N-phosphonate derivatives as corrosion inhibitor for mild steel in acid environment. <i>Surfaces and Interfaces</i> , 2020, 21, 100773.	1.5	15
10672	Photochemical and photophysical properties of cis-stilbene molecule by electronic structure calculations and nonadiabatic surface-hopping dynamics simulations. <i>Chemical Physics</i> , 2020, 539, 110957.	0.9	7
10673	Modeling Excited-State Proton Transfer to Solvent: A Dynamics Study of a Super Photoacid with a Hybrid Implicit/Explicit Solvent Model. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7033-7043.	2.3	26
10674	Structural evolution from exohedral to endohedral geometries, dynamical fluxionality, and structural forms of medium-sized anionic and neutral Au ₂ Si _n (n = 8–20) clusters. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25606-25617.	1.3	0
10675	Models and corrections: Range separation for electronic interaction—Lessons from density functional theory. <i>Journal of Chemical Physics</i> , 2020, 153, 160901.	1.2	12
10676	Optical and photovoltaic properties of substituted alizarin dyes for dye-sensitized solar cells application. <i>Energy Sources, Part A: Recovery, Utilization and Environmental Effects</i> , 0, , 1-14.	1.2	3
10677	Theoretical Study of the Dynamics of the HBr + CO ₂ → HOCO + Br Reaction. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9119-9127.	1.1	10
10678	Metal-organic magnets with large coercivity and ordering temperatures up to 242 Å°C. <i>Science</i> , 2020, 370, 587-592.	6.0	91
10679	Layer-dependent optoelectronic properties of black phosphorus. <i>International Journal of Modern Physics C</i> , 2020, 31, 2050177.	0.8	3
10680	Electron Spin Resonance of Defects in Spin Chains—A Versatile System Behaving Like Molecular Magnet. <i>Applied Magnetic Resonance</i> , 2020, 51, 1307-1320.	0.6	3
10681	Critical Role of Protons for Emission Quenching of Indoline Dyes in Solution and on Semiconductor Surfaces. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21346-21356.	1.5	9
10682	A mechanochemical model for the simulation of molecules and molecular crystals under hydrostatic pressure. <i>Journal of Chemical Physics</i> , 2020, 153, 134503.	1.2	16
10683	Fused polycyclic compounds: Synthesize, enhancing TPA cross-section by modifying torsional multiple ring. <i>Optical Materials</i> , 2020, 110, 110417.	1.7	2
10684	Electrochemical preparation and physicochemical study of polymers obtained from carbazole and N-((methoxycarbonyl)methyl)carbazole. <i>Synthetic Metals</i> , 2020, 270, 116584.	2.1	10
10685	Detection of NO _x and CO _x (x = 1, 2) molecules with T4,4,4-graphyne: a density functional theory study. <i>Molecular Simulation</i> , 2020, 46, 1383-1389.	0.9	5
10686	DFT counterparts of leading generalized gradient approximation and hybrid density functionals for energetics and geometries. <i>Journal of Computational Chemistry</i> , 2020, 41, 2562-2572.	1.5	61
10687	Bouncing off walls—widths of exit channels from shallow minima can dominate selectivity control. <i>Chemical Science</i> , 2020, 11, 9937-9944.	3.7	17
10688	Molecular insight into the anion effect and free volume effect of CO ₂ solubility in multivalent ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20618-20633.	1.3	27

#	ARTICLE	IF	CITATIONS
10689	Dinuclear Rhenium Complexes with a Bridging Helicene- π -bis(2,2'-bipyridine) Ligand: Synthesis, Structure, and Photophysical and Chiroptical Properties. <i>ChemPlusChem</i> , 2020, 85, 2446-2454.	1.3	7
10690	Computational Study of Anthracene-Based Organic Dyes for Dye-Sensitized Solar Cells: Effects of Auxiliary Electron Donors. <i>Journal of Electronic Materials</i> , 2020, 49, 6317-6324.	1.0	0
10691	Synthesis, Isolation, and Characterization of a Phenylsulfane-Selenolate Compound. <i>Inorganic Chemistry</i> , 2020, 59, 13315-13319.	1.9	2
10692	What is the Optimal Size of the Quantum Region in Embedding Calculations of Two-Photon Absorption Spectra of Fluorescent Proteins?. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6439-6455.	2.3	6
10693	Charge-Transfer Excitation Energies Expressed as Orbital Energies of Kohn-Sham Density Functional Theory with Long-Range Corrected Functionals. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8079-8087.	1.1	14
10694	Accurate Computation of the Absorption Spectrum of Chlorophyll <i>a</i> with Pair Natural Orbital Coupled Cluster Methods. <i>Journal of Physical Chemistry B</i> , 2020, 124, 8761-8771.	1.2	65
10695	ReaxFF Reactive Molecular Dynamics Simulations of Mechano-Chemical Decomposition of Perfluoropolyether Lubricants in Heat-Assisted Magnetic Recording. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22496-22505.	1.5	17
10696	pK _a -Yay: A Black-Box Method Using Density Functional Theory and Implicit Solvation Models to Compute Aqueous pK _a Values of Weak and Strong Acids. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9061-9074.	1.1	9
10697	Ladder-type bithiophene imide-based organic semiconductors: understanding charge transport mechanisms in organic field effect transistors. <i>Journal of Materials Chemistry C</i> , 2020, 8, 15759-15770.	2.7	6
10698	Theoretical prediction of ¹³ C NMR spectrum of mixed triglycerides by mean of GIAO calculations to improve vegetable oils analysis. <i>Chemistry and Physics of Lipids</i> , 2020, 232, 104973.	1.5	8
10699	Degradation mechanism of trans-2-hexenal in the atmosphere. <i>Chemical Physics Letters</i> , 2020, 759, 138039.	1.2	4
10700	Shining light on the electronic structure and relaxation dynamics of the isolated oxyluciferin anion. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19022-19032.	1.3	5
10701	Lilypad aggregation: localised self-assembly and metal sequestration at a liquid-vapour interface. <i>Chemical Science</i> , 2020, 11, 7501-7510.	3.7	5
10702	Chiral Molecules as Sensitive Probes for Direct Detection of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \langle \text{mml:mi mathvariant="script"} \rangle P \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ -Odd Cosmic Fields. <i>Physical Review Letters</i> , 2020, 125, 123004.	2.9	15
10707	Periodic Solids and Electron Bands. , 2020, , 81-108.		0
10708	Uniform Electron Gas and sp-Bonded Metals. , 2020, , 109-128.		0
10709	Density Functional Theory: Foundations. , 2020, , 129-144.		0
10710	The Kohn-Sham Auxiliary System. , 2020, , 145-170.		0

#	ARTICLE	IF	CITATIONS
10711	Functionals for Exchange and Correlation I. , 2020, , 171-187.		0
10712	Functionals for Exchange and Correlation II. , 2020, , 188-214.		0
10713	Electronic Structure of Atoms. , 2020, , 215-229.		0
10714	Pseudopotentials. , 2020, , 230-258.		0
10716	Plane Waves and Grids: Basics. , 2020, , 262-282.		0
10717	Plane Waves and Real-Space Methods: Full Calculations. , 2020, , 283-294.		0
10718	Localized Orbitals: Tight-Binding. , 2020, , 295-319.		0
10719	Localized Orbitals: Full Calculations. , 2020, , 320-331.		0
10720	Augmented Functions: APW, KKR, MTO. , 2020, , 332-364.		0
10721	Augmented Functions: Linear Methods. , 2020, , 365-385.		0
10722	Locality and Linear-Scaling O(N) Methods. , 2020, , 386-410.		0
10723	Quantum Molecular Dynamics (QMD). , 2020, , 411-426.		0
10724	Response Functions: Phonons and Magnons. , 2020, , 427-445.		0
10725	Excitation Spectra and Optical Properties. , 2020, , 446-464.		0
10726	Surfaces, Interfaces, and Lower-Dimensional Systems. , 2020, , 465-480.		0
10727	Wannier Functions. , 2020, , 481-498.		0
10728	Polarization, Localization, and Berry Phases. , 2020, , 499-516.		0
10729	Topology of the Electronic Structure of a Crystal: Introduction. , 2020, , 517-530.		0

#	ARTICLE	IF	CITATIONS
10730	Two-Band Models: Berry Phase, Winding, and Topology. , 2020, , 531-546.		0
10731	Topological Insulators I: Two Dimensions. , 2020, , 547-568.		0
10732	Topological Insulators II: Three Dimensions. , 2020, , 569-580.		0
10751	Evaluation of Local Hybrid Functionals for Electric Properties: Dipole Moments and Static and Dynamic Polarizabilities. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8346-8358.	1.1	15
10752	Tuning the UV spectrum of PAHs by means of different N-doping types taking pyrene as paradigmatic example: categorization via valence bond theory and high-level computational approaches. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22003-22015.	1.3	10
10753	Ruthenium(II)-Catalyzed Homocoupling of $\hat{\pm}$ -Carbonyl Sulfoxonium Ylides Under Mild Conditions: Methodology Development and Mechanistic DFT Study. <i>Frontiers in Chemistry</i> , 2020, 8, 648.	1.8	3
10754	Accurate Hybrid Density Functionals with UW12 Correlation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6176-6194.	2.3	5
10755	A DFT Protocol for the Prediction of ^{31}P NMR Chemical Shifts of Phosphine Ligands in First-Row Transition-Metal Complexes. <i>Organometallics</i> , 2020, 39, 3121-3130.	1.1	15
10756	Co-Amorphization of Kanamycin with Amino Acids Improves Aerosolization. <i>Pharmaceutics</i> , 2020, 12, 715.	2.0	12
10757	Theoretical Study of VX Hydrolysis Mechanism Catalyzed by Phosphotriesterase Mutant H254R. <i>ChemistrySelect</i> , 2020, 5, 8986-8991.	0.7	2
10758	Open-shell donor-acceptor conjugated metal-free dyes for dye-sensitized solar cells. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 1477-1490.	1.7	9
10759	White hyperelectrofluorescence from solution-processable OLEDs based on phenothiazine substituted tetraphenylethylene derivatives. <i>Journal of Materials Chemistry C</i> , 2020, 8, 13375-13388.	2.7	37
10760	Nuclear Quantum Effect on the Geometry of $\text{NH}_4^+(\text{H}_2\text{O})$. <i>Bulletin of the Chemical Society of Japan</i> , 2020, 93, 1558-1563.	2.0	3
10761	Naphthalene Benzimidazole Based Neutral Ir(III) Emitters for Deep Red Organic Light-Emitting Diodes. <i>Inorganic Chemistry</i> , 2020, 59, 12461-12470.	1.9	16
10762	Assessing the Tamm-Dancoff approximation, singlet-singlet, and singlet-triplet excitations with the latest long-range corrected double-hybrid density functionals. <i>Journal of Chemical Physics</i> , 2020, 153, 064106.	1.2	54
10763	Temperature-dependent changes in the molecular orientation and visible color of phthalocyanine films. <i>RSC Advances</i> , 2020, 10, 31348-31354.	1.7	1
10764	Thiazol-2-thiolate-Bridged Binuclear Platinum(II) Complexes with High Photoluminescence Quantum Efficiencies of up to Near Unity. <i>Inorganic Chemistry</i> , 2020, 59, 13109-13116.	1.9	29
10765	Understanding Enzyme Catalysis Mechanism Using QM/MM Simulation Methods. <i>ACS Symposium Series</i> , 2020, , 121-137.	0.5	1

#	ARTICLE	IF	CITATIONS
10766	Analysis of Ion Pairing in Solid State and Solution in <i>p</i> -Cymene Ruthenium Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 14171-14183.	1.9	8
10767	Understanding the luminescence properties of Cu(<i>scp</i>) complexes: a quantum chemical perusal. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23530-23544.	1.3	33
10768	Parity-nonconserving interactions of electrons in chiral molecules with cosmic fields. <i>Physical Review A</i> , 2020, 102, .	1.0	4
10769	Density Functional Theory Calculation and Raman Scattering of the Antihistamine Ebastine. <i>Journal of Applied Spectroscopy</i> , 2020, 87, 608-614.	0.3	4
10770	Single or Paired? Structure and Reactivity of PNP-Chromium(II) Hydrides. <i>Inorganic Chemistry</i> , 2020, 59, 14526-14535.	1.9	9
10771	Towards developing efficient metalloporphyrin-based hybrid photocatalysts for CO ₂ reduction; an ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23128-23140.	1.3	5
10772	Understanding the <i>g</i> -tensors of perchlorotriphenylmethyl and Finland-type trityl radicals. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20792-20800.	1.3	9
10773	Computational Discovery of Stable Heteroanionic Oxychalcogenides ABXO (A, B = Metals; X = S, Se, and Te). <i>Journal of Physical Chemistry A</i> , 2020, 124, 7795-7804.	1.1	10
10774	Computation of Molecular Electron Affinities Using an Ensemble Density Functional Theory Method. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7795-7804.	1.1	10
10775	Nicotinonitrile centered luminescent polymeric materials: Structural, optical, electrochemical, and theoretical investigations. <i>Polymer Engineering and Science</i> , 2020, 60, 2550-2559.	1.5	8
10776	Tailoring desolvation kinetics enables stable zinc metal anodes. <i>Journal of Materials Chemistry A</i> , 2020, 8, 19367-19374.	5.2	136
10777	15N NMR Shifts of Eumelanin Building Blocks in Water: A Combined Quantum Mechanics/Statistical Mechanics Approach. <i>Molecules</i> , 2020, 25, 3616.	1.7	3
10778	Comparison of 1,2-Diarylcyclopropanecarboxylates with 1,2,2-Triarylcyclopropanecarboxylates as Chiral Ligands for Dirhodium-Catalyzed Cyclopropanation and C-H Functionalization. <i>Journal of Organic Chemistry</i> , 2020, 85, 12199-12211.	1.7	12
10779	Intriguing Radical-Radical Interactions in Doubly Reduced Dimers: Cytosine Anion Radical versus Hydrogenated Cytosine Radical. <i>Journal of Physical Chemistry C</i> , 2020, 124, 19760-19773.	1.5	1
10780	Computation of Dipole Moments: A Recommendation on the Choice of the Basis Set and the Level of Theory. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7538-7548.	1.1	25
10781	The electronic and spectroscopic investigation of (±)-Dasycarpidone. <i>Vibrational Spectroscopy</i> , 2020, 111, 103156.	1.2	24
10782	Machine learning the Hubbard U parameter in DFT+U using Bayesian optimization. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	80
10783	Rapid Sequentially Palladium Catalyzed Four-Component Synthesis of Novel Fluorescent Biaryl-Substituted Isoxazoles. <i>Catalysts</i> , 2020, 10, 1412.	1.6	5

#	ARTICLE	IF	CITATIONS
10784	Computer simulation of collision induced dissociation and isolobal analogy: The case of biotin and its analogs. <i>International Journal of Mass Spectrometry</i> , 2020, 457, 116417.	0.7	0
10785	Nonparametric Local Pseudopotentials with Machine Learning: A Tin Pseudopotential Built Using Gaussian Process Regression. <i>Journal of Physical Chemistry A</i> , 2020, 124, 11111-11124.	1.1	10
10786	9,10-Anthraquinones Disubstituted with Linear Alkoxy Groups: Spectroscopy, Electrochemistry, and Peculiarities of Their 2D and 3D Supramolecular Organizations. <i>Langmuir</i> , 2020, 36, 15048-15063.	1.6	11
10787	Synthesis, <i>in vitro</i> anticancer activities, and quantum chemical investigations on 1,3-bis-(2-methyl-2-propenyl)benzimidazolium chloride and its Ag(I) complex. <i>Journal of Chemical Research</i> , 2021, 45, 596-607.	0.6	4
10788	Doping Capabilities of Fluorine on the UV Absorption and Emission Spectra of Pyrene-Based Graphene Quantum Dots. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10954-10966.	1.1	9
10789	Amino Acid Replacement at Position 228 Induces Fluctuation in the α_1 -Loop of KPC-3 and Reduces the Affinity against Oxyimino Cephalosporins: Kinetic and Molecular Dynamics Studies. <i>Catalysts</i> , 2020, 10, 1474.	1.6	1
10790	Benzene- and pyridine-incorporated octaphyrins with different coordination modes toward two PdII centers. <i>Nature Communications</i> , 2020, 11, 6206.	5.8	16
10791	Adiabatic connection in spin-current density functional theory. <i>Physical Review B</i> , 2020, 102, .	1.1	16
10792	Pure Rotational Spectrum of Benzophenone Detected by Broadband Microwave Spectrometer in the 2â€“8 GHz Range. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 8471.	1.3	1
10793	Synthesis, Structure and Physical Properties of (trans-TTF-py ₂) _{1.5} (PF ₆) ₃ ·EtOH: A Molecular Conductor with Weak CHâ€“â€“N Hydrogen Bondings. <i>Crystals</i> , 2020, 10, 1081.	1.0	2
10794	Photoinduced Electron Injection in a Fully Solvated Dye-Sensitized Photoanode: A Dynamical Semiempirical Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 27965-27976.	1.5	11
10795	10-Methylthiocolchicine complexes with lithium, sodium, potassium, rubidium and cesium metal cations salts â€“ Cytotoxic, semi-empirical and molecular modelling studies. <i>Polyhedron</i> , 2020, 190, 114791.	1.0	1
10796	How CuI and NaI Interact with Faujasite Zeolite? A Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2020, 124, 28026-28037.	1.5	2
10797	Photodynamic activity attained through the ruptured π -conjugation of pyridyl groups with a porphyrin macrocycle: synthesis and the photophysical and photobiological evaluation of 5-mono-(4-nitrophenyl)-10,15,20-tris-[4-(phenoxy)methyl]pyridine]porphyrin and its Zn(II) complex. <i>Photochemical and Photobiological Sciences</i> , 2020, 19, 1776-1789.	1.6	3
10798			

#	ARTICLE	IF	CITATIONS
10802	Vacuum-Ultraviolet Absorption Spectrum of 3-Methoxyacrylonitrile. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9470-9477.	1.1	6
10803	Rotational spectra of van der Waals complexes: pyrrole-Ne and pyrrole-Ne ₂ . <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25652-25660.	1.3	9
10804	Identification and Reactivity of <i>cis</i> - <i>cis</i> - <i>cis</i> -Dihydroxycarbene, a New [CH ₂ O ₂] Intermediate. <i>Journal of the American Chemical Society</i> , 2020, 142, 19457-19461.	6.6	5
10805	The Modification of Poly(metal phosphates) by Pentaerythritol. <i>Polymer Science - Series B</i> , 2020, 62, 534-539.	0.3	1
10806	Mechanistic Studies of Hydrogen Evolution Reaction on Donor-Acceptor Conjugated Polymer Photocatalysts. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 7017.	1.3	5
10807	Physical Fundamentals of Biomaterials Surface Electrical Functionalization. <i>Materials</i> , 2020, 13, 4575.	1.3	11
10808	Solid-State Electron Affinity Analysis of Amorphous Fluorinated Polymer Electret. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10507-10513.	1.2	8
10809	Optoelectronic and thermal properties of cubic SiMO ₃ (M = Sn, Pb) oxides for device application: a first principle study. <i>Optical and Quantum Electronics</i> , 2020, 52, 1.	1.5	3
10810	Reaction mechanisms and topological analyses for the C-H activation of ethylene by uranium atom using density functional theory. <i>Computational and Theoretical Chemistry</i> , 2020, 1190, 113022.	1.1	1
10811	Mechanistic Studies of Nickel-Catalyzed Hydroarylation of Styrenes. <i>Organic Letters</i> , 2020, 22, 8998-9003.	2.4	22
10812	Computational refinement of the puzzling red tetrasulfur chromophore in ultramarine pigments. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22684-22698.	1.3	9
10813	Two-dimensional diamine-linked covalent organic frameworks for CO ₂ /N ₂ capture and separation: theoretical modeling and simulations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25918-25929.	1.3	16
10814	Origin invariant optical rotation in the length dipole gauge without London atomic orbitals. <i>Journal of Chemical Physics</i> , 2020, 153, 151101.	1.2	17
10815	Structures and Stability of Complexes of E(C ₆ F ₅) ₃ (E = B, Al, Ga). <i>Tj ETQq1 0.0.784314 rgBT / Ov</i>	1.0	9
10816	Iridium catalysts featuring amine-containing ligands for the dehydrogenation of formic acid. <i>Journal of Organometallic Chemistry</i> , 2020, 916, 121259.	0.8	3
10817	The one-electron self-interaction error in 74 density functional approximations: a case study on hydrogenic mono- and dinuclear systems. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15805-15830.	1.3	27
10818	Structural, spectroscopic and electronic properties of a family of face-shared bi-octahedral Ru ₂ ^{+5/6+} complexes with a bridging 2,5-di(2-pyridyl)pyrrolide ligand. <i>Dalton Transactions</i> , 2020, 49, 7053-7059.	1.6	2
10819	One-bond ¹ J(¹⁵ N,H) coupling constants at sp ² -hybridized nitrogen of Schiff bases, enamines and similar compounds: A theoretical study. <i>Magnetic Resonance in Chemistry</i> , 2020, 58, 750-762.	1.1	4

#	ARTICLE	IF	CITATIONS
10820	On the Discrepancy between Experimental and Calculated Raman Intensities for Conjugated Phenyl and Thiophene Derivatives. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4678-4689.	1.1	7
10821	Heteroleptic Samarium(III) Chalcogenide Complexes: Opportunities for Giant Exchange Coupling in Bridging f- and f-Radical Lanthanide Dichalcogenides. <i>Inorganic Chemistry</i> , 2020, 59, 7571-7583.	1.9	14
10822	Microscopic Link between Electron Localization and Chemical Expansion in AMnO ₃ and ATiO ₃ Perovskites (A = Ca, Sr, Ba). <i>Journal of Physical Chemistry C</i> , 2020, 124, 12922-12932.	1.5	12
10823	Theoretical investigation on the Cu(II)-catalyzed N-carboxamidation of indoles with isocyanates to form indole-1-carboxamides: effects of solvents. <i>New Journal of Chemistry</i> , 2020, 44, 9878-9887.	1.4	2
10824	Performance of density functional theory and orbital-optimised second-order perturbation theory methods for geometries and singlet-triplet state splittings of aryl-carbenes. <i>Molecular Physics</i> , 2020, 118, e1764644.	0.8	19
10825	N-Cobalt(II) Pincer Complexes: Paramagnetic NMR Spectroscopy in Solution and Application as Hydrosilylation Catalysts. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 2335-2342.	1.0	16
10826	Computation of Molecular Ionization Energies Using an Ensemble Density Functional Theory Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4489-4504.	2.3	8
10827	Self-Assembly Properties of Solution Processable, Electroactive Alkoxy, and Alkylthienylene Derivatives of Fused Benzoacridines: A Scanning Tunneling Microscopy Study. <i>Langmuir</i> , 2020, 36, 5417-5427.	1.6	3
10828	Solvatochromism of a Novel Ruthenium Complex, [Ru(acac) ₂ (N-(2-Methylsulfonylphenyl)formamido)]: A Correlation between the Electronic Structure and Spectroscopic Properties. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 789-799.	0.1	0
10829	Extra-Terrestrial Gas-Phase Stereoinversion in Amino Acid Leucine: Thermal and Photochemical Channels. <i>ChemPhysChem</i> , 2020, 21, 1107-1118.	1.0	3
10830	Structural studies of 3-tert-butyl-8-(methylchalcogenyl)pyrazolo[5,1-c][1,2,4]triazin-4(1H)-ones. <i>Structural Chemistry</i> , 2020, 31, 1457-1470.	1.0	11
10831	Mechanism, kinetics, and environmental assessment of OH-initiated transformation of CTDE in the atmosphere. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26250.	1.0	1
10832	Solvent Mediated Excited State Proton Transfer in Indigo Carmine. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4156-4162.	2.1	26
10833	Diketopyrrolopyrrole-based multifunctional ratiometric fluorescent probe and β -glutamyltranspeptidase-triggered activatable photosensitizer for tumor therapy. <i>Journal of Materials Chemistry C</i> , 2020, 8, 8183-8190.	2.7	26
10834	Investigating the Sulfur Twist on the Photophysics of DBD Dyes. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4345-4353.	1.1	3
10835	Mechanism of antioxidant properties of quercetin and quercetin-DNA complex. <i>Journal of Molecular Modeling</i> , 2020, 26, 133.	0.8	53
10836	Electron Spin Densities and Density Functional Approximations: Open-Shell Polycyclic Aromatic Hydrocarbons as Case Study. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3567-3577.	2.3	20
10837	A new tuned range-separated density functional for the accurate calculation of second hyperpolarizabilities. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11871-11880.	1.3	28

#	ARTICLE	IF	CITATIONS
10838	Fully numerical calculations on atoms with fractional occupations and range-separated exchange functionals. <i>Physical Review A</i> , 2020, 101, .	1.0	22
10839	Triarylboron/Triarylamine-Functionalized 2,2'-Bipyridine Ligands and Their Copper(I) Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 7426-7434.	1.9	11
10840	Size Dependence of [C _n]Cycloparaphenylenes (C _n = 9-20): Relationship between Aromaticity and Third-Order Nonlinear Optical Properties. <i>Journal of Physical Chemistry C</i> , 2020, 124, 11081-11091.	1.5	16
10841	Insight into the effects of the donors and pi-spacers on the photovoltaic performance of quinoline and pyridocarbazole based DSSCs. <i>Optical Materials</i> , 2020, 106, 109974.	1.7	13
10842	Do HOMO-LUMO Energy Levels and Band Gaps Provide Sufficient Understanding of Dye-Sensitizer Activity Trends for Water Purification?. <i>ACS Omega</i> , 2020, 5, 15052-15062.	1.6	18
10843	Insights into interactions of Cr(III) and organic matters during adsorption onto titanate nanotubes: Differential absorbance and DFT study. <i>Journal of Molecular Liquids</i> , 2020, 312, 113432.	2.3	13
10844	Synthesis, crystal structure, experimental and theoretical studies of corrosion inhibition of 2-((4-(2-hydroxy-4-methylbenzyl)piperazin-1-yl)methyl)-5-methylphenol - A Mannich base. <i>Journal of Molecular Structure</i> , 2020, 1219, 128539.	1.8	28
10845	Band alignment at the CaF ₂ /Si interface through advanced electronic structure calculations. <i>Physical Review B</i> , 2020, 101, .		
10846	Nanoatomic scale hydrophobic/philic confinement of peptides on mineral surfaces by cross-correlated SPM and quantum mechanical DFT analysis. <i>Journal of Microscopy</i> , 2020, 280, 204-221.	0.8	7
10847	Novel gamma arsenene nanosheets as sensing medium for vomiting agents: A first-principles research. <i>Computational and Theoretical Chemistry</i> , 2020, 1185, 112876.	1.1	24
10848	Novel thiazoline-phenothiazine based push-pull molecules as fluorescent probes for volatile acids detection. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 397, 112509.	2.0	13
10849	Exploring the Reaction Mechanism of H ₂ S Decomposition with MS ₃ (M = Mo,) Tj ETQq1 1.0.784314 rgBT / Ov	1.6	14
10850	A search for the physical basis of the genetic code. <i>BioSystems</i> , 2020, 195, 104148.	0.9	3
10851	Effects of Noncovalent Interactions on High-Spin Fe(IV)-Oxido Complexes. <i>Journal of the American Chemical Society</i> , 2020, 142, 11804-11817.	6.6	53
10852	Direct deposition GC/IR techniques in natural product identification. <i>Natural Product Reports</i> , 2020, 37, 1561-1567.	5.2	7
10853	On the metal ion selectivity of PNP-ariat ether-an insight from density functional theory calculations. <i>Structural Chemistry</i> , 2020, 31, 1801-1819.	1.0	0
10854	Dibenzoylbenzodipyrroles: Key Precursors for the Synthesis of Fused meso-Aryl Sapphyrins. <i>Journal of Organic Chemistry</i> , 2020, 85, 7287-7296.	1.7	5
10855	Synthesis, Structure, and Optical Properties of Di-m-benzihexaphyrins (1.1.0.0.0.0) and Di-m-benziheptaphyrins (1.0.1.0.0.0.0): Blackening of m-Phenylene-Linked Dicarbaporphyrinoids by Simple Expansion. <i>Journal of Organic Chemistry</i> , 2020, 85, 8021-8028.	1.7	7

#	ARTICLE	IF	CITATIONS
10856	Density Functional Theory Study of the Metal-Catalyzed Cycloaddition of Indolyl-Allenenes: Possible Reaction Pathways, Stereoselectivity, and Regioselectivity. <i>Organometallics</i> , 2020, 39, 1782-1789.	1.1	7
10857	An sp-hybridized all-carboatomic ring, cyclo[18]carbon: Bonding character, electron delocalization, and aromaticity. <i>Carbon</i> , 2020, 165, 468-475.	5.4	188
10858	Theoretical investigation of the adsorption behaviors of fluorouracil as an anticancer drug on pristine and B-, Al-, Ga-doped C36 nanotube. <i>Journal of Molecular Liquids</i> , 2020, 309, 113209.	2.3	43
10859	An ab initio/RRKM study of the reaction mechanism and product branching ratios of CH3OH+ and CH3OH++ dissociation. <i>Journal of Molecular Structure</i> , 2020, 1217, 128410.	1.8	4
10860	Monitoring the Reactivity of Formamide on Amorphous SiO2 by In-Situ UV-Raman Spectroscopy and DFT Modeling. <i>Molecules</i> , 2020, 25, 2274.	1.7	3
10861	Interaction studies of aniline on pristine and Al-doped μ -Arsenene nanosheets – A first-principles insight. <i>Chemical Physics Letters</i> , 2020, 752, 137588.	1.2	36
10862	The inclusion behavior of 8-Anilino-1-naphthalene sulfonate into Cucurbit[7]uril: A DFT approach. <i>Journal of Molecular Structure</i> , 2020, 1217, 128390.	1.8	4
10863	Furanyl chalcone derivatives as efficient singlet oxygen quenchers. An experimental and DFT/MRCI study. <i>Tetrahedron</i> , 2020, 76, 131248.	1.0	3
10864	Theoretical Mechanistic Studies of Rh-Catalyzed C(sp ³)-H Amination: A Comparison with Co Analogue and Metal Effects. <i>Chinese Journal of Chemistry</i> , 2020, 38, 1526-1532.	2.6	4
10865	Synthesis, experimental and theoretical characterization of (E)-2-((2,3-dimethylphenyl)amino)-N-(furan-2-ylmethylene)benzohydrazide. <i>Journal of Molecular Structure</i> , 2020, 1219, 128518.	1.8	12
10866	Construction of Two-Dimensional Potential Energy Surfaces of Reactions with Post-Transition-State Bifurcations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4050-4060.	2.3	15
10867	Construction of frustrated Lewis pair from nitride and phosphine for the activation and cleavage of molecular hydrogen. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5811.	1.7	0
10868	Computational Assessment of Counterion Effect of Borate Anions on Ethylene Polymerization by Zirconocene and Hafnocene Catalysts. <i>Organometallics</i> , 2020, 39, 2068-2079.	1.1	18
10869	Achieving Site-Selectivity for C-H Activation Processes Based on Distance and Geometry: A Carpenter's Approach. <i>Journal of the American Chemical Society</i> , 2020, 142, 10571-10591.	6.6	236
10870	Exact Generalized Kohn-Sham Theory for Hybrid Functionals. <i>Physical Review X</i> , 2020, 10, .	2.8	19
10871	Triquinoline- versus Fullerene-Based Cycloparaphenylene Ionic Complexes: Comparison of Photoinduced Charge-Shift Reactions. <i>Chemistry - A European Journal</i> , 2020, 26, 10896-10902.	1.7	10
10872	Pd immobilization on the multi-amine functionalized halloysite as an efficient catalyst for hydrogenation reaction: An experimental and computational study. <i>Applied Clay Science</i> , 2020, 192, 105645.	2.6	19
10873	Band Gap in Magnetic Insulators from a Charge Transition Level Approach. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3786-3798.	2.3	22

#	ARTICLE	IF	CITATIONS
10874	Relationships between Orbital Energies, Optical and Fundamental Gaps, and Exciton Shifts in Approximate Density Functional Theory and Quasiparticle Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4337-4350.	2.3	21
10875	A Semiempirical Method to Detect and Correct DFT-Based Gas-Phase Errors and Its Application in Electrocatalysis. <i>ACS Catalysis</i> , 2020, 10, 6900-6907.	5.5	71
10876	Efficient C-H Amination Catalysis Using Nickel-Dipyrrin Complexes. <i>Journal of the American Chemical Society</i> , 2020, 142, 10996-11005.	6.6	66
10877	BNB-Doped Phenalenyls: Modular Synthesis, Optoelectronic Properties, and One-Electron Reduction. <i>Journal of the American Chemical Society</i> , 2020, 142, 11072-11083.	6.6	63
10878	A topological semimetal Li ₂ CrN ₂ sheet as a promising hydrogen storage material. <i>Nanoscale</i> , 2020, 12, 12106-12113.	2.8	9
10879	Microwave-Assisted Synthesis of Zirconium Phosphate Nanoplatelet-Supported Ru-Anadem Nanostructures and Their Catalytic Study for the Hydrogenation of Acetophenone. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 30670-30679.	4.0	10
10880	Hardware efficient quantum algorithms for vibrational structure calculations. <i>Chemical Science</i> , 2020, 11, 6842-6855.	3.7	50
10881	Probing Solute-Solvent Interactions of Transition Metal Complexes Using L-Edge Absorption Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5636-5645.	1.2	8
10882	Modelling the enthalpy change and transition temperature dependence of the metal-insulator transition in pure and doped vanadium dioxide. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13474-13478.	1.3	12
10883	Improvements in the orbitalwise scaling down of Perdew-Zunger self-interaction correction in many-electron regions. <i>Journal of Chemical Physics</i> , 2020, 152, 174112.	1.2	23
10884	Experimental and calculated second harmonic generation of a guanidinium salt in the solid state. <i>Solid State Communications</i> , 2020, 314-315, 113853.	0.9	0
10885	Quantum-Chemically Informed Machine Learning: Prediction of Energies of Organic Molecules with 10 to 14 Non-hydrogen Atoms. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5804-5811.	1.1	28
10886	Kinetic Investigations of the Reaction of Phenyl Radicals with Ethyl Acetate in the Gas Phase: An Experimental and Computational Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5503-5512.	1.1	7
10887	Ab initio description of nanodiamonds: A DFT and TDDFT benchmark. <i>Diamond and Related Materials</i> , 2020, 108, 107959.	1.8	10
10888	Cooperative bonding interactions of various oxygen species on the IB group metal anions. <i>International Journal of Mass Spectrometry</i> , 2020, 451, 116312.	0.7	4
10889	The Nanostructure of HMT-PMBI, a Sterically Hindered Ionene. <i>Macromolecules</i> , 2020, 53, 4908-4916.	2.2	4
10890	The role of interaction between low molecular weight neutral organic compounds and a polyamide RO membrane in the rejection mechanism. <i>RSC Advances</i> , 2020, 10, 15642-15649.	1.7	9
10891	Photoelectron spectra and electronic structure of boron diacetate formazanates. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 238, 118441.	2.0	4

#	ARTICLE	IF	CITATIONS
10892	Mg ²⁺ -Dependent Methyl Transfer by a Knotted Protein: A Molecular Dynamics Simulation and Quantum Mechanics Study. <i>ACS Catalysis</i> , 2020, 10, 8058-8068.	5.5	15
10893	Efficient Synthesis, SC-XRD, and Theoretical Studies of <i>O</i> -Benzenesulfonylated Pyrimidines: Role of Noncovalent Interaction Influence in Their Supramolecular Network. <i>ACS Omega</i> , 2020, 5, 15115-15128.	1.6	65
10894	Differentiating the role of organic additives to assemble open framework aluminosilicates using INS spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14177-14186.	1.3	1
10895	Computational Study of Methane C-H Activation by Main Group and Mixed Main Group Transition Metal Complexes. <i>Molecules</i> , 2020, 25, 2794.	1.7	2
10896	In Silico Design of Cylindrophanes: The Role of Functional Groups in a Fluoride Selective Host. <i>ChemPhysChem</i> , 2020, 21, 1989-2005.	1.0	5
10897	The aromatic fullerene-like silicon cage with 12 Si ₅ pentagons stabilized by a V ₃ unit. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	6
10898	Unexpected rapid aerobic transformation of 2,2,6,6-tetraethyl-4-oxo(piperidin-1-yloxy) radical by cytochrome P450 in the presence of NADPH: Evidence against a simple reduction of the nitroxide moiety to the hydroxylamine. <i>Free Radical Biology and Medicine</i> , 2020, 156, 144-156.	1.3	4
10899	Synthesis, crystal structure, hirshfeld surface analysis, DFT computations and molecular dynamics study of 2-(benzyloxy)-3-phenylquinoxaline. <i>Journal of Molecular Structure</i> , 2020, 1221, 128727.	1.8	14
10900	Sensitive detection of iron (II) sulfate with a novel reagent using spectrophotometry. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 240, 118631.	2.0	3
10901	Identifying the existence and molecular structure of the dissolved HCO ₃ -Ca-As(V) complex in water. <i>Science of the Total Environment</i> , 2020, 724, 138216.	3.9	3
10902	Theoretical Study on Chemiluminescence of H ₂ O ₂ -dependent Tetrachloro-1,4-benzoquinone. <i>Journal of Organic Chemistry</i> , 2020, 85, 9042-9050.	1.7	10
10903	Water Inhibition of Oxymethylene Dimethyl Ether Synthesis over Zeolite H-Beta: A Combined Kinetic and <i>in Situ</i> ATR-IR Study. <i>ACS Catalysis</i> , 2020, 10, 8106-8119.	5.5	20
10904	Encapsulation of Hydrogen Molecules in C ₅₀ Fullerene: An <i>ab Initio</i> Study of Structural, Energetic, and Electronic Properties of H ₂ @C ₅₀ and 2H ₂ @C ₅₀ Complexes. <i>ACS Omega</i> , 2020, 5, 12853-12864.	1.6	6
10905	Hydrogen bond interactions of hydrated aluminum nitrate with <i>PVDF</i> , <i>PVDF-TrFE</i> , and <i>PVDF-HFP</i> : A density functional theory-based illustration. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26328.	1.0	13
10906	Not only AIE: Light-sensitivity of 4-dimethylamino-2-hydroxychalcones beneficial to highly efficient photochemical synthesis of 4-dimethylaminoflavanones. <i>Journal of Molecular Liquids</i> , 2020, 313, 113526.	2.3	7
10907	Neutral excitation density-functional theory: an efficient and variational first-principles method for simulating neutral excitations in molecules. <i>Scientific Reports</i> , 2020, 10, 8947.	1.6	13
10908	More efficient spin-orbit coupling: adjusting the ligand field strength to the second metal ion in asymmetric binuclear platinum(<i>ii</i>) configurations. <i>Dalton Transactions</i> , 2020, 49, 8722-8733.	1.6	14
10909	A Comparative Study of Redox Mediators for Improved Performance of Li-Oxygen Batteries. <i>Advanced Energy Materials</i> , 2020, 10, 2000201.	10.2	32

#	ARTICLE	IF	CITATIONS
10910	SERS-based trace-level quantification of sulindac: Spectroscopic and molecular modeling evaluation. <i>Journal of Molecular Liquids</i> , 2020, 312, 113402.	2.3	21
10911	Solution Thermodynamics for the Thorium Complexation with N-(2-Hydroxyethyl) Iminodiacetic Acid. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 2927-2937.	1.0	8
10912	Carboxylate-Assisted \hat{I}^2 -(<i>Z</i>) Stereoselective Hydrosilylation of Terminal Alkynes Catalyzed by a Zwitterionic Bis-NHC Rhodium(III) Complex. <i>ACS Catalysis</i> , 2020, 10, 7367-7380.	5.5	24
10913	Interaction of K ₂ CrO ₄ Oxide Nanoparticles with Carbon Nanostructures. , 2020, , .		0
10914	DFT study of electronic and optical properties of nickel doped barium titanate nanostructures. <i>AIP Conference Proceedings</i> , 2020, , .	0.3	0
10915	Synthesis and Conformational Analysis of Naphthoxazine-Fused Phenanthrene Derivatives. <i>Molecules</i> , 2020, 25, 2524.	1.7	2
10916	Ground and Excited States of Gas-Phase DNA Nucleobase Cation-Radicals. A UV-vis Photodissociation Action Spectroscopy and Computational Study of Adenine and 9-Methyladenine. <i>Journal of the American Society for Mass Spectrometry</i> , 2020, 31, 1271-1281.	1.2	18
10917	Ligand architectural effect on coordination, bonding, interaction, and selectivity of Am(^{III}) and Ln(^{III}) ions with bitopic ligands: synthesis, solvent extraction, and DFT studies. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15448-15462.	1.3	13
10918	Thermoplastic Polycomplexes of Metal Phosphate and Primary Amines. <i>Russian Journal of Physical Chemistry B</i> , 2020, 14, 318-322.	0.2	3
10919	Efficient structural modification of electron-withdrawing substituents on Pt(II) complexes for red emitters: A theoretical study. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5739.	1.7	3
10920	Compact Basis Sets for Optical Rotation Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4408-4415.	2.3	13
10921	Domain Separated Density Functional Theory for Reaction Energy Barriers and Optical Excitations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5954-5962.	1.1	0
10922	Extrapolating Unconverged GW Energies up to the Complete Basis Set Limit with Linear Regression. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4399-4407.	2.3	14
10923	Spin-orbit coupling in periodic systems with broken time-reversal symmetry: Formal and computational aspects. <i>Physical Review B</i> , 2020, 101, .	1.1	24
10924	Phosphorus-Containing Dibenzonaphthanthrenes: Electronic Fine Tuning of Polycyclic Aromatic Hydrocarbons through Organophosphorus Chemistry. <i>Chemistry - A European Journal</i> , 2020, 26, 13157-13162.	1.7	15
10926	Accurate real-time evolution of electron densities and ground-state properties from generalized Kohn-Sham theory. <i>Physical Review A</i> , 2020, 101, .	1.0	3
10927	Detailed molecular structure (XRD), conformational search, spectroscopic characterization (IR,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 10 analogue. <i>Heliyon</i> , 2020, 6, e04106.	1.4	25
10928	New boron-capped cage manganese(II) complex with terminal thiophene-2-carboxaldehyde groups: Crystal structure and density functional theory investigation for electron transfer. <i>Journal of Molecular Structure</i> , 2020, 1219, 128481.	1.8	2

#	ARTICLE	IF	CITATIONS
10929	Interaction of light with a non-covalent zinc porphyrin-graphene oxide nanohybrid. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13456-13466.	1.3	19
10930	Investigation on adsorption properties of HCN and ClCN blood agents on phosphorene nanosheets: A first-principles insight. <i>Chemical Physics</i> , 2020, 538, 110896.	0.9	34
10931	Electronic structures and bonding of graphdiyne and its BN analogs: Transition from quasi-planar to planar sheets. <i>Journal of Alloys and Compounds</i> , 2020, 846, 155987.	2.8	5
10932	Experimental and theoretical investigations of the [Ln(² -dik)(NO ₃) ₂ (phen) ₂] ⁺ ·H ₂ O luminescent complexes. <i>Journal of Luminescence</i> , 2020, 226, 117455.	1.5	13
10933	Learning how planarization can affect dichroic patterns in polyfluorenes. <i>Chirality</i> , 2020, 32, 661-666.	1.3	4
10934	A computational study on multiple formaldehyde complexes and their possible chemical reactions as well as the catalytic effect in the gas phase. <i>SN Applied Sciences</i> , 2020, 2, 1.	1.5	1
10935	Reactivity Parameters and Substitution Effect in Organic Acids. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3770-3777.	1.1	5
10936	Tunable carbocation-based redox active ambiphilic ligands: synthesis, coordination and characterization. <i>Dalton Transactions</i> , 2020, 49, 16095-16105.	1.6	19
10937	Hydrogen-Bonded Small-Molecular Crystals Yielding Strong Ferroelectric and Antiferroelectric Polarizations. <i>Journal of the Physical Society of Japan</i> , 2020, 89, 051009.	0.7	51
10938	Effect of the Counterion on Circularly Polarized Luminescence of Europium(III) and Samarium(III) Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 5050-5062.	1.9	25
10939	Assessing model-dielectric-dependent hybrid functionals on the antiferromagnetic transition-metal monoxides MnO, FeO, CoO, and NiO. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 015502.	0.7	30
10940	Boosting Electrocatalytic N ₂ Reduction to NH ₃ over Two-Dimensional Gallium Selenide by Defect-Size Engineering. <i>Inorganic Chemistry</i> , 2020, 59, 4858-4867.	1.9	44
10941	Opening up the Valence Shell: A C ₆ -Shaped Iron(I) Metalloradical and Its Potential for Atom Abstraction. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 9448-9452.	7.2	21
10942	Synthesis, characterization and thermal properties of 1,10-phenanthroline mixed-ligand complexes of cobalt(II) and copper(II): metal-mediated transformations of the dicyanamide ion. <i>Chemical Papers</i> , 2020, 74, 3003-3016.	1.0	10
10943	Evaluation of Influencing Factors in Tetravalent Uranium Complex-Mediated CO ₂ Functionalization by Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2683-2693.	1.1	2
10944	Plane-wave many-body corrections to the conductance in bulk tunnel junctions. <i>Physical Review B</i> , 2020, 101, .	1.1	1
10946	Intermetallic Nanocatalysts from Heterobimetallic Group 10-14 Pyridine-2-thiolate Precursors. <i>Organometallics</i> , 2020, 39, 1092-1104.	1.1	11
10947	An Overview of Self-Consistent Field Calculations Within Finite Basis Sets. <i>Molecules</i> , 2020, 25, 1218.	1.7	37

#	ARTICLE	IF	CITATIONS
10948	Rotational and vibrational analysis of astrophysically relevant isomeric species of proteinogenic glutamic acid: A quantum-mechanical computational study. <i>Journal of Molecular Spectroscopy</i> , 2020, 369, 111271.	0.4	1
10949	Synthesis, solvent interactions and computational study of monocarbohydrazones. <i>Chemical Papers</i> , 2020, 74, 2653-2674.	1.0	2
10950	A synergistic synthetic and computational insights towards anomerization of N-nitro pyrimidine nucleosides using fluorinating agents. <i>Journal of Fluorine Chemistry</i> , 2020, 233, 109504.	0.9	0
10951	A rational design of excellent light-absorbing dyes with different N-substituents at the phenothiazine for high efficiency solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 234, 118241.	2.0	17
10952	Cl-Initiated Photo-oxidation Studies of Methyl Valerate and Methyl Isovalerate under Tropospheric Relevant Conditions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2515-2529.	1.1	0
10953	Molecular generation targeting desired electronic properties <i>via</i> deep generative models. <i>Nanoscale</i> , 2020, 12, 6744-6758.	2.8	27
10954	Performance of TDDFT Vertical Excitation Energies of Core-Substituted Naphthalene Diimides. <i>Journal of Computational Chemistry</i> , 2020, 41, 1448-1455.	1.5	21
10955	Density Functional Computations of Vibrational Circular Dichroism Spectra beyond the Born-Oppenheimer Approximation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2627-2634.	2.3	7
10956	Nonadiabatic Dynamics Simulations on Early-Time Photochemistry of Spirobenzopyran. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2547-2559.	1.1	16
10957	Probing the strong magnetic exchange behaviour of transition metal-radical complexes: a DFT case study. <i>Dalton Transactions</i> , 2020, 49, 4539-4548.	1.6	8
10958	Arsenic(III) complexes of substituted diphenyldithiophosphate: synthesis, characterization, single crystal X-ray, DFT, and Hirshfeld surface analysis. <i>Journal of Coordination Chemistry</i> , 2020, 73, 467-484.	0.8	1
10959	A possible alternative therapy for type 2 diabetes using <i>Myristica fragrans</i> Houtt in combination with glimepiride: in vivo evaluation and in silico support. <i>Zeitschrift Fur Naturforschung - Section C Journal of Biosciences</i> , 2020, 75, 103-112.	0.6	3
10960	Identification and in silico prediction of metabolites of tebufenozide derivatives by major human cytochrome P450 isoforms. <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115429.	1.4	0
10961	Novel μ -phosphorene nanosheet device for the detection of tear gas molecules – A first-principles research. <i>Chemical Physics Letters</i> , 2020, 747, 137353.	1.2	40
10962	Öffnung der Valenzschale: Ein σ -armiges Eisen(I)-Metalloradikal und sein Potential als Atomabstraktor. <i>Angewandte Chemie</i> , 2020, 132, 9535-9539.	1.6	4
10963	A zeroth-order active-space frozen-orbital embedding scheme for multireference calculations. <i>Journal of Chemical Physics</i> , 2020, 152, 094107.	1.2	10
10964	Density Functional Study of Cubic, Tetragonal, and Orthorhombic CsPbBr ₃ Perovskite. <i>ACS Omega</i> , 2020, 5, 7468-7480.	1.6	105
10965	A Digital Workflow Supporting the Selection of Solvents for Optimizing the Crystallizability of <i>p</i> -Aminobenzoic Acid. <i>Organic Process Research and Development</i> , 2020, 24, 500-507.	1.3	18

#	ARTICLE	IF	CITATIONS
10966	Effect of the linkage modes of thiolated ethynyl groups on the spin-dependent electronic transport properties in transition metal porphyrin molecular junctions. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 055301.	0.7	0
10967	Goldâ€“Carbon Contacts from Oxidative Addition of Aryl Iodides. <i>Journal of the American Chemical Society</i> , 2020, 142, 7128-7133.	6.6	31
10968	Chemical Equilibrium of Zinc Acetate Complexes in Ethanol Solution. A Theoretical Description through Thermodynamic Cycles. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3355-3370.	1.2	3
10969	Curcumin analogs as the inhibitors of TLR4 pathway in inflammation and their drug like potentialities: a computer-based study. <i>Journal of Receptor and Signal Transduction Research</i> , 2020, 40, 324-338.	1.3	19
10970	Visible Light-Induced Homolytic Cleavage of Perfluoroalkyl Iodides Mediated by Phosphines. <i>Molecules</i> , 2020, 25, 1606.	1.7	19
10971	Visualization of the Borazine Core of B ₃ N ₃ -Doped Nanographene by STM. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 19218-19225.	4.0	15
10972	Density functional theory study on the donating strength of donor systems in dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2020, 44, 7200-7209.	1.4	28
10973	The interplay of conformations and electronic properties in <i>N</i> -aryl phenothiazines. <i>Organic Chemistry Frontiers</i> , 2020, 7, 1206-1217.	2.3	38
10974	Revisiting the reactivity between HCO and CH ₃ on interstellar grain surfaces. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 493, 2523-2527.	1.6	25
10975	Mechanistic study on the effects of co-catalyst on ethylene polymerization over supported vanadocene catalyst. <i>Molecular Catalysis</i> , 2020, 486, 110852.	1.0	5
10976	Halomethane Adsorption Studies on Silicane Sheets: A First-Principles Perception. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2020, 30, 3263-3275.	1.9	16
10977	Bidentate Schiff Base Ligands Appended Metal(II) Complexes as Probes of DNA and Plasma Protein: In Silico Molecular Modelling Studies. <i>Applied Biochemistry and Biotechnology</i> , 2020, 191, 1515-1532.	1.4	14
10978	Density Function Theory calculation, and phthalonitrile process for a synthesis of single crystal zinc phthalocyanine. <i>Materials Science in Semiconductor Processing</i> , 2020, 113, 105025.	1.9	4
10979	Atmospheric chemical loss processes of isocyanic acid (HNCO): a combined theoretical kinetic and global modelling study. <i>Atmospheric Chemistry and Physics</i> , 2020, 20, 6671-6686.	1.9	12
10980	Spectroscopy driven DFT computation for a structure of the monomeric Cu ²⁺ -Curcumin complex and thermodynamics driven evaluation of its binding to DNA: Pseudo-binding of Curcumin to DNA. <i>Journal of Molecular Structure</i> , 2020, 1221, 128732.	1.8	6
10981	Comparison between Benzothiadizoleâ€“Thiophene- and Benzothiadizoleâ€“Furan-Based Dâ€“Aâ€“iâ€“A Dyes Applied in Dye-Sensitized Solar Cells: Experimental and Theoretical Insights. <i>ACS Omega</i> , 2020, 5, 16856-16864.	1.6	21
10982	Mechanistic insights of adenine promoted activity of low-molecule tyrosine phosphatase: An ONIOM study. <i>Chemical Physics Letters</i> , 2020, 754, 137719.	1.2	1
10983	Computational modeling of piezochromism in molecular crystals. <i>Journal of Chemical Physics</i> , 2020, 152, 234106.	1.2	4

#	ARTICLE	IF	CITATIONS
10984	Quantum Chemical Computations, Molecular Docking, Experimental and DFT Calculation of 4-Amino-3-Phenylbutanoic Acid. <i>Polycyclic Aromatic Compounds</i> , 2022, 42, 1302-1321.	1.4	5
10985	Microwave-Assisted Neat Synthesis of a Ferrocene Appended Phenolphthalein Diyne: A Designed Synthetic Scaffold for Hg ²⁺ Ion. <i>Inorganic Chemistry</i> , 2020, 59, 10099-10112.	1.9	10
10986	Relative contributions of Franck-Condon to Herzberg-Teller terms in charge transfer surface-enhanced Raman scattering spectroscopy. <i>Journal of Chemical Physics</i> , 2020, 152, 224107.	1.2	13
10987	Synthesis, characterization, and computational modeling of 6,6'-(((2-hydroxyethyl)azanediyl)bis(methylene))bis(2,4-di-tert-butylphenol) modified group 4 metal alkoxides. <i>Journal of Coordination Chemistry</i> , 2020, 73, 1389-1406.	0.8	1
10988	Modifying Phosphorus(III) Substituents to Activate Remote Ligand-Centered Reactivity in Triaminoborane Ligands. <i>Organometallics</i> , 2020, 39, 2526-2533.	1.1	5
10989	Active Catalyst for Methane Hydroxylation by an Iridium-Oxo Complex. <i>ACS Catalysis</i> , 2020, 10, 8254-8262.	5.5	4
10990	Rational design of 9-vinyl-phenyl noscapine as potent tubulin binding anticancer agent and evaluation of the effects of its combination on Docetaxel. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 5276-5289.	2.0	12
10991	Thermal hybrid exchange-correlation density functional for improving the description of warm dense matter. <i>Physical Review B</i> , 2020, 101, .	1.1	16
10992	Density Functionals for Hydrogen Storage: Defining the H2Bind275 Test Set with Ab Initio Benchmarks and Assessment of 55 Functionals. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4963-4982.	2.3	14
10993	The Catalytic Role of a Conserved Tyrosine in Nitric Oxide-Reducing Non-heme Diiron Enzymes. <i>ACS Catalysis</i> , 2020, 10, 8177-8186.	5.5	11
10994	Theoretical characterization of Al(III) binding to KSPVPKSPVEEK: Insights into the propensity of aluminum to interact with key sequences for neurofilament formation. <i>Journal of Inorganic Biochemistry</i> , 2020, 210, 111169.	1.5	1
10995	Synthesis, crystal structure, hirshfeld surface analysis, spectroscopic, biological and first-principles studies of novel aminocoumarins. <i>Journal of Molecular Structure</i> , 2020, 1221, 128862.	1.8	28
10996	DFT Outlook on Surface Adsorption Properties of Nitrobenzene on Novel Red Tricycle Arsenene Nanoring. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2020, 30, 4329-4341.	1.9	16
10997	Quantitative evaluation of transient valence orbital occupations in a 3d transition metal complex as seen from the metal and ligand perspective. <i>Chemical Physics Letters</i> , 2020, 754, 137681.	1.2	6
10998	Difficulties of Popular Density Functionals to Describe the Conformational Isomerism in Iodoacetic Acid. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5570-5579.	1.1	2
10999	Density Functional Theory Investigation of Some Pyridine Dicarboxylic Acids Derivatives as Corrosion Inhibitors. <i>International Journal of Electrochemical Science</i> , 2020, 15, 4274-4286.	0.5	14
11000	Molecular Fluorescent Probes for Imaging and Evaluation of Hypochlorite Fluctuations during Diagnosis and Therapy of Osteoarthritis in Cells and in a Mouse Model. <i>ACS Sensors</i> , 2020, 5, 1949-1958.	4.0	71
11001	Mechanical force-induced manipulation of electronic conductance in a spin-crossover complex: a simple approach to molecular electronics. <i>Nanoscale Advances</i> , 2020, 2, 2907-2913.	2.2	11

#	ARTICLE	IF	CITATIONS
11002	Synthesis, characterization and electroluminescence studies of cyanopyridine-based π -conjugative polymers carrying benzo[1,2,5]thiadiazole and naphtho[1,2-c:5,6-c']bis([1,2,5]thiadiazole) units. <i>New Journal of Chemistry</i> , 2020, 44, 10796-10805.	1.4	8
11003	Electronic and optical properties of nickel doped potassium titanate nanostructures: A DFT study. <i>AIP Conference Proceedings</i> , 2020, . .	0.3	0
11004	Using electronegativity and hardness to test density functionals. <i>Journal of Chemical Physics</i> , 2020, 152, 244113.	1.2	5
11005	On the use of DFT+U to describe the electronic structure of TiO ₂ nanoparticles: (TiO ₂) ₃₅ as a case study. <i>Journal of Chemical Physics</i> , 2020, 152, 244107.	1.2	7
11006	Extending the ASS1ST Active Space Selection Scheme to Large Molecules and Excited States. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4993-5005.	2.3	19
11007	Fragmentation Mechanism of White Phosphorus: A Theoretical Insight into Multiple Cleavage/Formation of P-P and P-C Bonds. <i>Chemistry - A European Journal</i> , 2020, 26, 13282-13287.	1.7	13
11008	Fe-quaterpyridine complex: a comprehensive DFT study on the mechanism of CO ₂ -to-CO conversion. <i>Journal of Materials Science</i> , 2020, 55, 14301-14314.	1.7	3
11009	Solvent polarity effects on thermochemical and NMR parameters of spilanthalol pharmacological agent: an experimental and DFT investigation. <i>Structural Chemistry</i> , 2020, 31, 2281-2292.	1.0	2
11010	Promoting sensitivity and selectivity of NO ₂ gas sensor based on metal (Pt, Re, Ta)-doped monolayer WSe ₂ : A DFT study. <i>Chemical Physics Letters</i> , 2020, 755, 137737.	1.2	23
11011	Adsorption of NO ₂ on monolayer MoS ₂ doped with Fe, Co, and Ni, Cu: A computational investigation. <i>Chemical Physics Letters</i> , 2020, 755, 137768.	1.2	34
11012	Quantum chemical topology at the spin-orbit configuration interaction level: Application to astatine compounds. <i>Journal of Computational Chemistry</i> , 2020, 41, 2055-2065.	1.5	10
11013	Quantum chemical study of molecular properties of AsX _n (X = F and Cl, n = 1-5) and AsX _n ⁺ (X = F and Cl, n = 1-5). <i>Journal of Computational Chemistry</i> , 2020, 41, 2055-2065.	1.1	0.7843
11014	Soot inception: A DFT study of β and γ dimerization of resonantly stabilized aromatic radicals. <i>Fuel</i> , 2020, 279, 118491.	3.4	19
11015	Diastereoselective Synthesis of P-Stereogenic Secondary Phosphine Oxides (SPOs) Bearing a Chiral Substituent by Ring Opening of (+)-Limonene Oxide with Primary Phosphido Nucleophiles. <i>Journal of Organic Chemistry</i> , 2020, 85, 14516-14526.	1.7	8
11016	Origins of Unconventional β^3 Site Selectivity in Palladium-Catalyzed C(sp ³)-H Activation and Arylation of Aliphatic Alcohols. <i>Organic Letters</i> , 2020, 22, 1464-1468.	2.4	18
11017	Advances in the Molecular Catalysis of Dioxygen Reduction. <i>ACS Catalysis</i> , 2020, 10, 2640-2655.	5.5	76
11018	Electron-Transfer and Redox Reactivity of High-Valent Iron Imido and Oxo Complexes with the Formal Oxidation States of Five and Six. <i>Journal of the American Chemical Society</i> , 2020, 142, 3891-3904.	6.6	43
11019	Synthesis, characterization, computational and biological studies of nitrothiazole incorporated heterocyclic azo dyes. <i>Structural Chemistry</i> , 2020, 31, 1317-1329.	1.0	16

#	ARTICLE	IF	CITATIONS
11020	Elucidating the Electronic Structure of High-Spin [Mn ^{III} (TPP)Cl] Using Magnetic Circular Dichroism Spectroscopy. <i>Inorganic Chemistry</i> , 2020, 59, 2144-2162.	1.9	18
11021	Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function. <i>Journal of Chemical Physics</i> , 2020, 152, 054107.	1.2	35
11022	Competitive Reactivity of Tautomers in the Degradation of Organophosphates by Imidazole Derivatives. <i>Chemistry - A European Journal</i> , 2020, 26, 5017-5026.	1.7	9
11023	Rare-Earth Catalyzed C-H Bond Almination of Terminal Alkynes. <i>Chemistry - A European Journal</i> , 2020, 26, 5479-5493.	1.7	4
11024	Molecular-Level Mechanism of Phosphoric Acid Digestion of Carbonates and Recalibration of the ¹³ C/ ¹⁸ O Clumped Isotope Thermometer. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 420-433.	1.2	9
11025	Time-Domain Terahertz Spectroscopy and Density Functional Theory Studies of Nitro/Nitrogen-Rich Aryl-Tetrazole Derivatives. <i>ACS Omega</i> , 2020, 5, 2541-2551.	1.6	14
11026	Synthesis and electronic structure studies of a Cr-imido redox series. <i>Chemical Communications</i> , 2020, 56, 3163-3166.	2.2	11
11027	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. <i>Chemical Reviews</i> , 2020, 120, 2215-2287.	23.0	231
11028	Electronic Transport and Non-linear Optical Properties of Hexathiopentacene (HTP) Nanorings: A DFT Study. <i>Journal of Electronic Materials</i> , 2020, 49, 3282-3289.	1.0	13
11029	Performance of Electronic Structure Methods for the Description of H ₂ ckelâ€™MÃ¶bius Interconversions in Extended Î€-Systems. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2380-2397.	1.1	22
11030	First-Principle Insights Into Molecular Design for High-Voltage Organic Electrode Materials for Mg Based Batteries. <i>Frontiers in Chemistry</i> , 2020, 8, 83.	1.8	14
11031	Extension of Î€-conjugation and enhancement of electron-withdrawing ability at terminal indenedione for A-Î€-D-Î€-A small molecules for application in organic solar cells. <i>Organic Electronics</i> , 2020, 81, 105679.	1.4	10
11032	Large-Scale Parallel Implementation of Hartreeâ€™Fock Exchange Energy on Real-Space Grids Using 3D-Parallel Fast Fourier Transform. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1376-1389.	2.5	4
11033	Cyclometalated Pt Complexes of CNC Pincer Ligands: Luminescence and Cytotoxic Evaluation. <i>Organometallics</i> , 2020, 39, 746-756.	1.1	41
11034	Aminoalkyl radicals as halogen-atom transfer agents for activation of alkyl and aryl halides. <i>Science</i> , 2020, 367, 1021-1026.	6.0	285
11035	DFT study on the â€œSilver effectâ€•in gold-catalyzed hydroamination of terminal alkynyl sulfamides. <i>Molecular Catalysis</i> , 2020, 486, 110847.	1.0	2
11036	Benchmark of Simplified Time-Dependent Density Functional Theory for UVâ€™Vis Spectral Properties of Porphyrinoids. <i>Advanced Theory and Simulations</i> , 2020, 3, 1900192.	1.3	13
11037	A density functional theory study on the shape of the primary cellulose microfibril in plants: effects of C6 exocyclic group conformation and H-bonding. <i>Cellulose</i> , 2020, 27, 2389-2402.	2.4	29

#	ARTICLE	IF	CITATIONS
11038	Narrowing band gap and enhanced visible-light absorption of metal-doped non-toxic CsSnCl ₃ metal halides for potential optoelectronic applications. RSC Advances, 2020, 10, 7817-7827.	1.7	54
11039	Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials. Physical Review B, 2020, 101, .	1.1	43
11040	The tautomerism of imidazo[4,5-e]benzo[1,2-c,3,4-c] difuroxans: A quantum chemical and experimental study. Journal of Molecular Structure, 2020, 1207, 127775.	1.8	0
11041	The first examples of triply bonded dirhenium(II,II) complexes that contain bis(diphenylphosphino)methane and dithiocarbamate ligands: spectroscopic, structural, cytotoxicity and computational studies. New Journal of Chemistry, 2020, 44, 4081-4091.	1.4	8
11042	Flexibility of the CueR Metal Site Probed by Instantaneous Change of Element and Oxidation State from Ag ^I to Cd ^{II} . Chemistry - A European Journal, 2020, 26, 7451-7457.	1.7	10
11043	On the Surface Acid-Base Properties of Amorphous and Crystalline Mg ₂ SiO ₄ as Probed by Adsorbed CO, CO ₂ , and CD ₃ CN. ACS Earth and Space Chemistry, 2020, 4, 345-354.	1.2	5
11044	Isomer-specific cryogenic ion vibrational spectroscopy of the D ₂ tagged Cs ⁺ (HNO ₃)(H ₂ O) _{n=0-2} complexes: ion-driven enhancement of the acidic H-bond to water. Physical Chemistry Chemical Physics, 2020, 22, 4501-4507.	1.3	9
11045	Initial-state preparation effects in time-resolved electron paramagnetic resonance experiments. Journal of Chemical Physics, 2020, 152, 044304.	1.2	2
11046	Profiling C4N radicals of astrophysical interest. Monthly Notices of the Royal Astronomical Society, 2020, 493, 2506-2510.	1.6	8
11047	Colorimetric and smartphone-integrated paper device for on-site determination of arsenic (III) using sucrose modified gold nanoparticles as a nanoprobe. Mikrochimica Acta, 2020, 187, 173.	2.5	46
11048	Invited Review: Modern Methods for Accurately Simulating the Terahertz Spectra of Solids. Journal of Infrared, Millimeter, and Terahertz Waves, 2020, 41, 491-528.	1.2	35
11049	Synthetic and computational studies on Cu/ligand pair promoted activation of C(Aryl)-Cl bond in C-N coupling reactions. Heliyon, 2020, 6, e03233.	1.4	4
11050	Energetics of paramagnetic oxide clusters: the Fe(III) oxyhydroxy Keggin ion. Physical Chemistry Chemical Physics, 2020, 22, 4043-4050.	1.3	0
11051	Cyclic versus straight chain oligofuran as sensor: A detailed DFT study. Journal of Molecular Graphics and Modelling, 2020, 97, 107569.	1.3	66
11052	Spectroscopy characterization, theoretical study and antioxidant activities of the flavonoids-Pb(II) complexes. Journal of Molecular Structure, 2020, 1209, 127919.	1.8	22
11053	A review of investigation on 4-substituted 1,8-naphthalimide derivatives. Synthetic Metals, 2020, 262, 116328.	2.1	45
11054	Substitution tuned electronic absorption, charge transfer and non-linear optical properties of some D _{6h} A type 2,4,6-trisubstituted-1,3,5-triazines: a DFT study. Bulletin of Materials Science, 2020, 43, 1.	0.8	4
11055	Quantum chemical and kinetic study of the CCl ₂ +HCl→CHCl ₃ insertion reaction. Computational and Theoretical Chemistry, 2020, 1176, 112742.	1.1	4

#	ARTICLE	IF	CITATIONS
11056	A theoretical study on gas-phase reactions of acrylic acid with chlorine atoms: mechanism, kinetics, and insights. <i>Environmental Science and Pollution Research</i> , 2020, 27, 15772-15784.	2.7	5
11057	Chiral 1,5-disubstituted 1,2,3-triazoles – versatile tools for foldamers and peptidomimetic applications. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 1957-1967.	1.5	11
11058	Color-specific porosity in double pigmented natural 3d-nanoarchitectures of blue crab shell. <i>Scientific Reports</i> , 2020, 10, 3019.	1.6	21
11059	Shedding light on the bonding situation of triangular and square heterometallic clusters: computational insight. <i>New Journal of Chemistry</i> , 2020, 44, 5079-5087.	1.4	2
11060	Superconducting praseodymium superhydrides. <i>Science Advances</i> , 2020, 6, eaax6849.	4.7	99
11061	Towards an unified chemical model of secondary bonding. <i>Journal of Molecular Modeling</i> , 2020, 26, 62.	0.8	14
11062	Unusual Fluorescence Quenching-Based Al ³⁺ Sensing by an Imidazolylpiperazine Derivative. β -Cyclodextrin Encapsulation-Assisted Augmented Sensing. <i>Journal of Fluorescence</i> , 2020, 30, 445-453.	1.3	3
11063	Adsorption of small gas molecules on strained monolayer WSe ₂ doped with Pd, Ag, Au, and Pt: A computational investigation. <i>Applied Surface Science</i> , 2020, 514, 145911.	3.1	70
11064	Frequency and temperature dependent dielectric studies of propylene glycol-sulfolane binary mixtures in the microwave frequency region. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 233, 118189.	2.0	0
11065	Standard formation enthalpies of gas phase molecular complexes derived by taking into account the heat capacity difference of the gas phase dissociation processes: Experimental tensimetry data revisited. <i>Thermochimica Acta</i> , 2020, 686, 178571.	1.2	3
11066	Global Hybrid Multiconfiguration Pair-Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2274-2283.	2.3	15
11067	Extensive Quantum Chemistry Study of Neutral and Charged C ₄ N Chains: An Attempt To Aid Astronomical Observations. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 434-448.	1.2	8
11068	Interaction studies of kidney biomarker volatiles on black phosphorene nanoring: A first-principles investigation. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107566.	1.3	38
11069	The solvent effect on a styryl-bodipy derivative functioning as an AND molecular logic gate. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26181.	1.0	8
11070	Theoretical studies on the N–X (X = Cl, O) bond activation mechanism in catalytic C–H amination. <i>Catalysis Science and Technology</i> , 2020, 10, 1914-1924.	2.1	5
11071	Spectroscopic and computational study of a new thiazolylazonaphthol dye 1-[(5-(3-nitrobenzyl)-1,3-thiazol-2-yl)diazanyl]naphthalen-2-ol. <i>Journal of Molecular Liquids</i> , 2020, 304, 112713.	2.3	16
11072	Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based <i>Ab Initio</i> Molecular Dynamics. 1. Theory, Algorithm, and Performance. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3757-3785.	2.3	29
11073	O ₂ Activation by Non-Heme Thiolate-Based Dinuclear Fe Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 3249-3259.	1.9	17

#	ARTICLE	IF	CITATIONS
11074	Copper(I) catalyzed CO ₂ transformation: A density functional theory investigation. Computational and Theoretical Chemistry, 2020, 1175, 112745.	1.1	0
11075	Modulation of spin effect in electronic and vibrational properties of terbium dihydride (TbH ₂): An ab-initio study. International Journal of Hydrogen Energy, 2020, 45, 8783-8793.	3.8	3
11076	Rational Development of Remote C-H Functionalization of Biphenyl: Experimental and Computational Studies. Angewandte Chemie - International Edition, 2020, 59, 4770-4777.	7.2	39
11077	Clar Rules the Electronic Properties of 2D Conjugated Frameworks: Mind the Gap. Chemistry - A European Journal, 2020, 26, 6569-6575.	1.7	8
11078	Lock-and-Key Exciplexes for Thermally Activated Delayed Fluorescence. Organic Materials, 2020, 02, 001-010.	1.0	7
11079	Hydrogen-bond facilitated intramolecular proton transfer in excited state and fluorescence quenching mechanism of flavonoid compounds in aqueous solution. Journal of Molecular Liquids, 2020, 302, 112562.	2.3	34
11080	Facet-Independent Oxygen Evolution Activity of Pure \hat{I}^2 -NiOOH: Different Chemistries Leading to Similar Overpotentials. Journal of the American Chemical Society, 2020, 142, 3600-3612.	6.6	114
11081	Design of Lewis base functionalized ionic liquids for the N-formylation of amines with CO ₂ and hydrosilane: The cation effects. Catalysis Today, 2020, 356, 563-569.	2.2	29
11082	Synergistic Approach of Ultrafast Spectroscopy and Molecular Simulations in the Characterization of Intramolecular Charge Transfer in Push-Pull Molecules. Molecules, 2020, 25, 430.	1.7	24
11083	<i>Ab initio</i> calculations of the rate of carrier trapping and release at dopant sites in NaI: Tl beyond the harmonic approximation. Physical Review B, 2020, 101, .	1.1	2
11084	Unusual demetalation of iron from [2]ferrocenophane skeleton of dinuclear ferracycle carbonyl complex. Applied Organometallic Chemistry, 2020, 34, e5431.	1.7	1
11085	Stimuli-responsive phenothiazine-based donor-acceptor isomers: AIE, mechanochromism and polymorphism. Journal of Materials Chemistry C, 2020, 8, 3589-3602.	2.7	55
11086	Orbital localization error of density functional theory in shear properties of vanadium and niobium. Journal of Chemical Physics, 2020, 152, 024118.	1.2	8
11087	Radical attack and mineralization mechanisms on electrochemical oxidation of p-substituted phenols at boron-doped diamond anodes. Chemosphere, 2020, 248, 126033.	4.2	22
11088	DFT analysis of supra-molecular assemblies of substituted 4H-pyran derivatives. Journal of Molecular Structure, 2020, 1207, 127785.	1.8	3
11089	Why Purine Nucleoside Phosphorylase Ribosylates 2,6-Diamino-8-azapurine in Noncanonical Positions? A Molecular Modeling Study. Journal of Chemical Information and Modeling, 2020, 60, 1595-1606.	2.5	3
11090	The DFT Quest for Possible Reaction Pathways, Catalytic Species, and Regioselectivity in the InCl ₃ -Catalyzed Cycloaddition of N-Tosyl Formaldimine with Olefins or Allenes. Journal of Organic Chemistry, 2020, 85, 3676-3688.	1.7	7
11091	A Computational Strategy for the Design of Photochromic Derivatives Based on Diarylethene and Nickel Dithiolene with Large Contrast in Nonlinear Optical Properties. Journal of Physical Chemistry C, 2020, 124, 4221-4241.	1.5	23

#	ARTICLE	IF	CITATIONS
11092	Evidence That Molecules in Molecular Junctions May Not Be Subject to the Entire External Perturbation Applied to Electrodes. <i>Langmuir</i> , 2020, 36, 1329-1337.	1.6	5
11093	Preparation of an efficient catalyst through injection of CuI on modified poly (styrene-co-maleic) Tj ETQq1 1 0.784314 rgBT /Overl... <i>Applied Organometallic Chemistry</i> , 2020, 34, e5435.	1.7	4
11094	Insight into the Expanded Mislinked Porphyrins with High Second Order Nonlinear Optical Response. <i>Journal of Physical Chemistry A</i> , 2020, 124, 955-965.	1.1	18
11095	On the photophysical properties of IrIII, PtII, and PdII (phenylpyrazole) (phenyldipyrin) complexes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3217-3233.	1.3	17
11096	Roles of Base in the Pd-Catalyzed Annulative Chlorophenylene Dimerization. <i>ACS Catalysis</i> , 2020, 10, 3059-3073.	5.5	16
11097	Insights into the binding interaction of substrate with catechol 2,3-dioxygenase from biophysics point of view. <i>Journal of Hazardous Materials</i> , 2020, 391, 122211.	6.5	28
11098	Electrolyte-assisted dissolution-recrystallization mechanism towards high energy density and power density CF cathodes in potassium cell. <i>Nano Energy</i> , 2020, 70, 104552.	8.2	41
11099	Bis- and mixed-ligand copper(II) complexes of nalidixic acid the antibacterial drug: Mode of nalidixate coordination determines DNA binding and cleavage and cytotoxicity. <i>Inorganica Chimica Acta</i> , 2020, 504, 119450.	1.2	15
11100	Design, synthesis and application of triazole ligands in suzuki miyaura cross coupling reaction of aryl chlorides. <i>Journal of Molecular Structure</i> , 2020, 1206, 127753.	1.8	12
11101	Deep Red emitting dicyanovinylene isophorone based chromophores: Combined synthesis, optical properties, viscosity sensitivity, and DFT studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 391, 112389.	2.0	5
11102	Tuning Second-Order Nonlinear Optical Properties of Cross-Linked Carbon Nanotube via External Electric Field. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3778-3783.	1.5	10
11103	Rational Development of Remote C-H Functionalization of Biphenyl: Experimental and Computational Studies. <i>Angewandte Chemie</i> , 2020, 132, 4800-4807.	1.6	3
11104	Benzothiazole-pyridone and benzothiazole-pyrazole clubbed emissive azo dyes and dyeing application on polyester fabric: UPF, biological, photophysical and fastness properties with correlative computational assessments. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 230, 118064.	2.0	31
11105	Structure Reassignment of Echin sulfone A and the Echin sulfonic Acids A-D Supported by Single-Crystal X-ray Diffraction and Density Functional Theory Analysis. <i>Journal of Natural Products</i> , 2020, 83, 105-110.	1.5	14
11106	Structurally Isomerized Bis-Biphenyl Moieties Embedded in Hexaphyrin(3.1.1.3.1.1) and Octaphyrin(1.1.1.0.1.1.1.0). <i>Organic Letters</i> , 2020, 22, 1081-1085.	2.4	8
11107	Calculation of vibrationally resolved absorption and fluorescence spectra of the rylene. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2379-2385.	1.3	13
11108	3d-transition metals (Cu, Fe, Mn, Ni, V and Zn)-doped pentacene ĩ-conjugated organic molecule for photovoltaic applications: DFT and TD-DFT calculations. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	19
11109	Infrared-Assisted Synthesis of Prebiotic Glycine. <i>ChemPhysChem</i> , 2020, 21, 503-509.	1.0	3

#	ARTICLE	IF	CITATIONS
11110	A Novel Way to Enhance the Thermoelectric Efficiency of Carbon Nanotube through Cobaltocene- <i>decamethyl Cobaltocene Encapsulation</i> . <i>ChemistrySelect</i> , 2020, 5, 1539-1546.	0.7	1
11111	Excited-State Absorption by Linear Response Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4693-4700.	1.5	22
11112	What do we learn from the classical turning surface of the Kohn-Sham potential as electron number is varied continuously?. <i>Journal of Chemical Physics</i> , 2020, 152, 054105.	1.2	1
11113	Phthalocyanine-Cored Fluorophores with Fluorene-Containing Peripheral Two-Photon Antennae as Photosensitizers for Singlet Oxygen Generation. <i>Molecules</i> , 2020, 25, 239.	1.7	13
11114	How To Produce Methane Precursor in the Upper Ocean by An Untypical Non-Heme Fe-Dependent Methylphosphonate Synthase?. <i>ChemPhysChem</i> , 2020, 21, 385-396.	1.0	12
11115	A rotational study of the AlaAla dipeptide. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13867-13871.	1.3	10
11116	A simple D-A- π -A configured carbazole based dye as an active photo-sensitizer: A comparative investigation on different parameters of cell. <i>Journal of Molecular Liquids</i> , 2020, 310, 113189.	2.3	27
11117	Direct magnetic-field dependence of NMR chemical shift. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8485-8490.	1.3	4
11118	A newly synthesized green corrosion inhibitor imidazoline derivative for carbon steel in 7.5% NH ₄ Cl solution. <i>Sustainable Chemistry and Pharmacy</i> , 2020, 16, 100258.	1.6	14
11119	Stepwise Activation of Water by Open-Shell Interactions, Cl(H ₂ O) _n = 4-8,17. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3417-3437.	1.1	6
11120	Xe ⁻ OCS: relatively straightforward?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5615-5624.	1.3	4
11121	Lithium bis(oxalate)borate additive in the electrolyte to improve Li-rich layered oxide cathode materials. <i>Materials Chemistry Frontiers</i> , 2020, 4, 1689-1696.	3.2	33
11122	Predictions of solvation Gibbs free energies with COSMO-SAC approaches. <i>Fluid Phase Equilibria</i> , 2020, 517, 112614.	1.4	6
11123	Experimental and DFT studies on complexation of uranyl with N-(2-Hydroxyethyl)iminodiacetic acid in aqueous medium. <i>Inorganica Chimica Acta</i> , 2020, 508, 119653.	1.2	13
11124	Bayesian Optimization for Calibrating and Selecting Hybrid-Density Functional Models. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4053-4061.	1.1	107
11125	Electronic structure of bulk manganese oxide and nickel oxide from coupled cluster theory. <i>Physical Review B</i> , 2020, 101, .	1.1	27
11126	Mechanistic Insights into the Chemo-Selective Dehydrogenative Silylation of Alkenes Catalyzed by Bis(imino)pyridine Cobalt Complex from DFT Computations. <i>ChemCatChem</i> , 2020, 12, 3890-3899.	1.8	2
11127	Adamsite and chloropicrin molecular adsorption studies on novel green phosphorene nanotube - First-principles investigation. <i>Chemical Physics</i> , 2020, 535, 110782.	0.9	27

#	ARTICLE	IF	CITATIONS
11128	Benchmarking computational methods and influence of guest conformation on chirogenesis in zinc porphyrin complexes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11025-11037.	1.3	5
11129	MiMiC: Multiscale Modeling in Computational Chemistry. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 45.	1.6	5
11130	Status and Challenges of Density Functional Theory. <i>Trends in Chemistry</i> , 2020, 2, 302-318.	4.4	216
11131	Molecular dynamics simulation of the electron ionization mass spectrum of tabun. <i>Journal of Mass Spectrometry</i> , 2020, 55, e4513.	0.7	10
11132	Dissociative photoionization of 1,3-dioxolane: We need six channels to fit the elephant. <i>Journal of Mass Spectrometry</i> , 2020, 55, e4522.	0.7	6
11133	Multi-target heteroleptic palladium bisphosphonate complexes. <i>Journal of Biological Inorganic Chemistry</i> , 2020, 25, 509-519.	1.1	6
11134	N ₂ H ₂ binding to the nitrogenase FeMo cluster studied by QM/MM methods. <i>Journal of Biological Inorganic Chemistry</i> , 2020, 25, 521-540.	1.1	16
11135	DFT and TD-DFT studies of new pentacene-based organic molecules as a donor material for bulk-heterojunction solar cells. <i>Journal of Computational Electronics</i> , 2020, 19, 895-904.	1.3	19
11136	Syntheses, solution behavior, and computational bond length analyses of trifluoromethyl and perfluoroethyl cuprate salts. <i>Journal of Fluorine Chemistry</i> , 2020, 234, 109518.	0.9	5
11137	Assessing corrosion inhibition characteristics of hydrazone derivatives on mild steel in HCl: Insights from electronic-scale DFT and atomic-scale molecular dynamics. <i>Journal of Molecular Liquids</i> , 2020, 308, 112998.	2.3	71
11138	Electronic Structure and Magnetic Properties of a Titanium(II) Coordination Complex. <i>Inorganic Chemistry</i> , 2020, 59, 6187-6201.	1.9	7
11139	Theoretical study of the mechanism behind the site- and enantio-selectivity of C-H functionalization catalysed by chiral dirhodium catalyst. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9561-9572.	1.3	5
11140	Induced magnetic field in sp-hybridized carbon rings: analysis of double aromaticity and antiaromaticity in cyclo[2N]carbon allotropes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9240-9249.	1.3	46
11141	Slow magnetic relaxation and water oxidation activity of dinuclear Co ^{II} Co ^{III} and unique triangular Co ^{II} Co ^{II} Co ^{III} mixed-valence complexes. <i>Dalton Transactions</i> , 2020, 49, 6328-6340.	1.6	15
11142	Formation of silica-supported platinum nanoparticles as a function of preparation conditions and boron impregnation. <i>Journal of Chemical Physics</i> , 2020, 152, 134701.	1.2	3
11143	Novel Polycondensed Partly Saturated $\hat{1}^2$ -Carbolines Including Ferrocene Derivatives: Synthesis, DFT-Supported Structural Analysis, Mechanism of Some Diastereoselective Transformations and a Preliminary Study of their In Vitro Antiproliferative Effects. <i>Molecules</i> , 2020, 25, 1599.	1.7	1
11144	How accurate are TD-DFT excited-state geometries compared to DFT ground-state geometries?. <i>Journal of Computational Chemistry</i> , 2020, 41, 1718-1729.	1.5	57
11145	Thermoelectricity of n-type MnBi ₄ Se ₇ -7xSe _{7x} solid solution. <i>Chemical Engineering Journal</i> , 2020, 396, 125219.	6.6	8

#	ARTICLE	IF	CITATIONS
11146	Rhodium-Stabilized Diarylcarbenes Behaving as Donor/Acceptor Carbenes. <i>ACS Catalysis</i> , 2020, 10, 6240-6247.	5.5	43
11147	Weakly Coordinating Fluorine-Free Polysalt for Single Lithium-Ion Conductive Solid Polymer Electrolytes. <i>Batteries and Supercaps</i> , 2020, 3, 738-746.	2.4	14
11148	Photocatalytic dye degradation under sunlight irradiation using cerium ion adsorbed two-dimensional graphitic carbon nitride. <i>Journal of Environmental Chemical Engineering</i> , 2020, 8, 103942.	3.3	33
11149	First-principles study of bcc Fe-Cr-Si binary and ternary random alloys from special quasi-random structure. <i>Physica B: Condensed Matter</i> , 2020, 586, 412085.	1.3	8
11150	Establishing best practices to model the electronic structure of CuFeO from first principles. <i>Physical Review B</i> , 2020, 101, .		
11151	Substituted \hat{I}_{\pm} -Phenyl and \hat{I}_{\pm} -Naphthyl- <i>N</i> - <i>tert</i> -butyl Nitrones: Synthesis, Spin-Trapping, and Neuroprotection Evaluation. <i>Journal of Organic Chemistry</i> , 2020, 85, 6073-6085.	1.7	16
11152	Formation of $\text{Fe}(\text{OH})_3$ -As complexes: effect on the solubility of ferric hydroxide precipitates and molecular structural identification. <i>Environmental Science: Nano</i> , 2020, 7, 1388-1398.	2.2	9
11153	Hybrid functionals with system-dependent parameters: Conceptual foundations and methodological developments. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1476.	6.2	7
11154	New Chromenylium ⁺ cyanine based dual channel chemosensors for copper and hypochlorite sensing. <i>Dyes and Pigments</i> , 2020, 180, 108445.	2.0	16
11155	Synthesis, crystal structure, Hirshfeld surface analysis, spectral characterization, and quantum computational evaluation of (E)-2-(((4-bromophenyl)imino)methyl)-6-methylphenol. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 144, 109478.	1.9	5
11156	Molecular structure, aromaticity, vibrational investigation and dual descriptor for chemical reactivity on 1-chloroisoquinoline using quantum chemical studies. <i>Results in Materials</i> , 2020, 6, 100097.	0.9	8
11157	Thermodynamics and Structure of Neptunium(V) Complexes with Formate. <i>Spectroscopic and Theoretical Study</i> . <i>Inorganic Chemistry</i> , 2020, 59, 6067-6077.	1.9	6
11158	A Solid-State Luminescent Cd(II) Supramolecular Coordination Framework Based on Mixed Luminophores as a Sensor for Discriminatively Selective Detection of Amine Vapors. <i>Inorganic Chemistry</i> , 2020, 59, 6176-6186.	1.9	20
11159	Comparison of Spin-Flip TDDFT-Based Conical Intersection Approaches with XMS-CASPT2. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3253-3263.	2.3	12
11160	Investigating the (Poly)Radicaloid Nature of Real-World Organic Compounds with DFT-Based Methods. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3590-3600.	1.1	7
11161	Proton Transfer in Phosphoric Acid-Based Protic Ionic Liquids: Effects of the Base. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4141-4149.	1.1	6
11162	On the Spectroscopic Modeling of Localized Defects in Sodalites by TD-DFT. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8949-8957.	1.5	15
11163	Delocalization of the Excited State and Emission Spectrum of the Platinum(II) Bipyridine Complex in Crystal: Periodic QM/MM Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 10453-10461.	1.5	16

#	ARTICLE	IF	CITATIONS
11164	Silicon Forms a Rich Diversity of Aliphatic Polyol Complexes in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2020, 142, 9188-9202.	6.6	5
11165	Enhanced charge transport <i>via</i> $d(\pi)$ - $p(\pi)$ conjugation in Mo ₂ -integrated single-molecule junctions. <i>Nanoscale</i> , 2020, 12, 10320-10327.	2.8	10
11166	Electron correlation effects and magneto-optical properties of yttrium iron garnet. <i>AIP Advances</i> , 2020, 10, .	0.6	6
11167	Comparison and improvement of the predictability and interpretability with ensemble learning models in QSPR applications. <i>Journal of Cheminformatics</i> , 2020, 12, 19.	2.8	38
11168	A density functional theory study of the stereoselectivity of Cu(OTf) ₂ -catalyzed [3+2] cycloaddition of trifluoromethylated <i>N</i> -acylhydrazones and isoprene: A concerted asynchronous mechanism. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26236.	1.0	1
11169	The Activation Strain Model in the Light of Real Space Energy Partitions. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 1062-1072.	0.6	7
11170	Quantum chemical modeling of molecules under pressure. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26208.	1.0	14
11171	<i>Theae nigrae</i> folium: Comparing the analytical performance of benchtop and handheld near-infrared spectrometers. <i>Talanta</i> , 2021, 221, 121165.	2.9	39
11172	2-Hexylthiophene-substituted Alizarin-based (D π A) Organic Dyes for Dye-sensitized Solar Cell Applications: Density Functional Theory and UV-Vis Studies. <i>Journal of Chemical Research</i> , 2021, 45, 13-20.	0.6	2
11173	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of σ -SIE and σ -NCE. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, .	6.2	25
11174	The Trip to the Density Functional Theory Zoo Continues: Making a Case for Time-Dependent Double Hybrids for Excited-State Problems. <i>Australian Journal of Chemistry</i> , 2021, 74, 3.	0.5	39
11175	The influence of sorbitol doping on aggregation and electronic properties of PEDOT:PSS: a theoretical study. <i>Machine Learning: Science and Technology</i> , 2021, 2, 01LT01.	2.4	4
11176	Chemical reactivity theory (CRT) study of small drug-like biologically active molecules. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 943-952.	2.0	13
11177	Description of excited states in photochemistry with theoretical methods. <i>ChemistrySelect</i> , 2021, 6, .	0.7	2
11178	A computational quantum chemical and polarizability calculations of liquid crystal 4-cyano-4-pentylbiphenyl with water molecule (H ₂ O). <i>Journal of Molecular Structure</i> , 2021, 1227, 129568.	1.8	3
11179	Molecular dynamics simulation-directed rational design of nanoporous graphitic carbon nitride membranes for water desalination. <i>Journal of Membrane Science</i> , 2021, 620, 118869.	4.1	30
11180	Effect of non-ionic surfactants on the adsorption of polycyclic aromatic compounds at water/oil interface: A molecular simulation study. <i>Journal of Colloid and Interface Science</i> , 2021, 586, 766-777.	5.0	33
11181	pysisphus: Exploring potential energy surfaces in ground and excited states. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26390.	1.0	29

#	ARTICLE	IF	CITATIONS
11182	Identifying and explaining the regioselectivity of alkylation of 1,2,4-triazole-3-thiones using NMR, GIAO and DFT methods. <i>Journal of Molecular Structure</i> , 2021, 1223, 128973.	1.8	17
11183	Synthesis of bis[benzyl- λ^2 -hydrazinocarbodithioato- λ^2 , S]nickel(II) complex as a novel lead molecule for cancer treatment. <i>Applied Organometallic Chemistry</i> , 2021, 35, .	1.7	4
11184	Chemisorption of Heptachlor and Mirex molecules on beta arsenene nanotubes – A first-principles analysis. <i>Applied Surface Science</i> , 2021, 537, 147835.	3.1	32
11185	Microscopic mechanism about the selective adsorption of Cr(VI) from salt solution on O-rich and N-rich biochars. <i>Journal of Hazardous Materials</i> , 2021, 404, 124162.	6.5	63
11186	Adsorption behaviour of metronidazole drug molecule on the surface of hydrogenated graphene, boron nitride and boron carbide nanosheets in gaseous and aqueous medium: A comparative DFT and QTAIM insight. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 126, 114483.	1.3	58
11187	Simple 3,6-disubstituted Carbazoles as Potential Hole Transport Materials: Photophysical, Electrochemical and Theoretical Studies. <i>Photochemistry and Photobiology</i> , 2021, 97, 289-300.	1.3	13
11188	Quantification of Noncovalent Interactions in Azide-Pnictogen, Chalcogen, and Halogen Contacts. <i>Chemistry - A European Journal</i> , 2021, 27, 4627-4639.	1.7	25
11189	Experimental and computational studies of perillaldehyde isolated from <i>Ammodaucus leucotrichus</i> essential oil as a green corrosion inhibitor for mild steel in 1.0M HCl. <i>Chemical Papers</i> , 2021, 75, 1103-1114.	1.0	14
11190	Ab initio investigation of the ground and lowest excited states of the YAl molecule. <i>Computational and Theoretical Chemistry</i> , 2021, 1194, 113057.	1.1	0
11191	Building up Pt ^{II} -Thiosemicarbazone-Lysine's C18 Conjugates. <i>ChemBioChem</i> , 2021, 22, 694-704.	1.3	8
11192	Surface-induced dimerization of 2-thiazoline-2-thiol on silver and gold nanoparticles: A surface enhanced Raman scattering (SERS) and density functional theoretical (DFT) study. <i>Journal of Molecular Liquids</i> , 2021, 322, 114536.	2.3	13
11193	Ultra-smooth finishing of single-crystal lutetium oxide by plasma-assisted etching. <i>Precision Engineering</i> , 2021, 67, 77-88.	1.8	4
11194	A Raman spectroscopy and rheology study of the phase transitions of the ionic liquid choline acetate. <i>Journal of Molecular Liquids</i> , 2021, 322, 114530.	2.3	12
11195	Spectroscopic, molecular dynamics simulation and biological studies of Flavin MonoNucleotide and Flavin Adenine Dinucleotide in biomimetic systems. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 118997.	2.0	3
11196	The Size-Accelerated Kinetic Resolution of Secondary Alcohols. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 774-778.	7.2	17
11197	Enhancement of one- and two-photon absorption and visualization of intramolecular charge transfer of pyrenyl-contained derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 245, 118897.	2.0	26
11198	The shape selectivity of corannulene dimers based on concave-convex and convex-convex shape complementarity as hosts for C60 and C70. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 405-414.	1.3	8
11199	Inhibition of Urease, a N-Enzyme: The Reactivity of a Key Thiol With Mono- and Di-Substituted Catechols Elucidated by Kinetic, Structural, and Theoretical Studies. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 6029-6035.	7.2	12

#	ARTICLE	IF	CITATIONS
11200	Comparative study of the electronic and photocatalytic properties of bulk and monolayer MX ₂ : A TB-mBJ study. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 264, 114944.	1.7	14
11201	Tetraphenylbiphenyldiamine: Insight into anion storage mechanism as a cathode in dual ion batteries. <i>Applied Surface Science</i> , 2021, 542, 148581.	3.1	7
11202	DFT study on the [4+4] domino cycloaddition of ynones with benzylidenepyrazolones to access eight-membered cyclic ethers: effects of DBU vs. Et ₃ N. <i>New Journal of Chemistry</i> , 2021, 45, 131-140.	1.4	4
11203	Cataloguing the Energetic Contributions to the Supramolecular Assembly of para-Substituted N,N'-Diphenylureas and Their Organometallic Derivatives in the Solid State: A Density Functional Theory Approach. <i>Crystal Growth and Design</i> , 2021, 21, 563-571.	1.4	0
11204	Equilibrium, Thermodynamic, and Density Functional Theory Modeling Studies for the Removal of Dichromate Ions from Wastewater Using Calix[4]arene Modified Silica Resin. <i>Journal of Chemical & Engineering Data</i> , 2021, 66, 379-388.	1.0	9
11205	Bridge Substitution in DASAs: The Subtle Equilibrium between Photochemical Improvements and Thermal Control**. <i>Chemistry - A European Journal</i> , 2021, 27, 4420-4429.	1.7	10
11206	Toward coupling of electrochemical redox properties with electrostatic potential surfaces tailored by dopant architectures for pyrenetetrone. <i>Energy Storage Materials</i> , 2021, 35, 610-619.	9.5	15
11207	New naphthoquinone-imidazole hybrids: Synthesis, anion recognition properties, DFT studies and acid dissociation constants. <i>Journal of Molecular Liquids</i> , 2021, 327, 114855.	2.3	23
11208	First principle study of lithium and phosphorus co-doped graphitic carbon nitride as a nonlinear optical material. <i>Materials Today Communications</i> , 2021, 26, 101911.	0.9	4
11209	Interpretation of the formation of unstable halogen-containing disinfection by-products based on the differential absorbance spectroscopy approach. <i>Chemosphere</i> , 2021, 268, 129241.	4.2	3
11210	Structural Changes in Five-Coordinate Bromido-bis(o-aminobenzo-semiquinonato)iron(III) Complex: Spin-Crossover or Ligand-Metal Antiferromagnetic Interactions?. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 756-762.	1.0	1
11211	Structural and electronic properties of PtnSi12 (n=1-4) clusters: Quantum chemical calculations. <i>Computational and Theoretical Chemistry</i> , 2021, 1195, 113091.	1.1	1
11212	Theoretical design and characterization of D-A1-A based organic dyes for efficient DSSC by altering promising acceptor (A1) moiety. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 407, 113048.	2.0	28
11213	Tuning the donating strength of dye sensitizers using molecular electrostatic potential analysis. <i>New Journal of Chemistry</i> , 2021, 45, 2496-2507.	1.4	5
11214	Cation Radicals of Hachimoji Nucleobases P and Z: Generation in the Gas Phase and Characterization by UV-Vis Photodissociation Action Spectroscopy and Theory. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 373-386.	1.2	8
11215	Evidence of the presence of minor tautomeric forms in selected nitroanilines. <i>Rapid Communications in Mass Spectrometry</i> , 2021, 35, e9000.	0.7	1
11216	Synthesis, DFT computational insights on structural, optical, photoelectrical characterizations and spectroscopic parameters of the novel (2E)-3-(4-methoxy-5-oxo-5H-furo[3,2-b]pyridin-2-ylidene)-2-methylpropanoic acid (2-g) bromen-6-		
11217	Molecular structure and mild steel/HCl corrosion inhibition of 4,5-Dicyanoimidazole: Vibrational, electrochemical and quantum mechanical calculations. <i>Journal of Molecular Structure</i> , 2021, 1230, 129647.	1.8	43

#	ARTICLE	IF	CITATIONS
11218	Understanding the photophysics of stercobilin-Zn(II) and urobilin-Zn(II) complexes towards faecal pigment analysis. <i>Chemosphere</i> , 2021, 265, 129189.	4.2	6
11219	Reaction activity and mechanism of R3-CH structure oxidation in coal self-heating. <i>Fuel</i> , 2021, 290, 119797.	3.4	22
11220	An insight into non-covalent interactions in the tetraphenylarsonium dithiophosphates: Synthesis, DFT and Hirshfeld surface analysis. <i>Journal of Molecular Structure</i> , 2021, 1229, 129729.	1.8	7
11221	New cyanopyridine-based π -conjugative poly(azomethine)s: Synthesis, characterization and electroluminescence studies. <i>Polymers for Advanced Technologies</i> , 2021, 32, 131-141.	1.6	7
11222	Unraveling the catalytically preferential pathway between the direct and indirect hydrogenation of CO ₂ to CH ₃ OH using N-heterocyclic carbene-based Mn(i) catalysts: a theoretical approach. <i>Catalysis Science and Technology</i> , 2021, 11, 1375-1385.	2.1	13
11223	Tailoring the electronic and optical properties of layered blue phosphorene/ XC (X=Ge, Si) vdW heterostructures by strain engineering. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 127, 114460.	1.3	7
11224	Chemical enhancement effects on protoporphyrin IX surface-enhanced Raman spectra: Metal substrate dependence and a vibronic theory analysis. <i>Journal of Raman Spectroscopy</i> , 2021, 52, 323-338.	1.2	9
11225	Fundamental insights and rational design of low-cost polyoxometalates for the oxygen evolution reaction. <i>Journal of Catalysis</i> , 2021, 393, 202-206.	3.1	10
11226	Theoretical prediction of Xe-containing polymer. <i>Molecular Physics</i> , 2021, 119, e1842532.	0.8	0
11227	NH ₃ separation membranes with self-assembled gas highways induced by protic ionic liquids. <i>Chemical Engineering Journal</i> , 2021, 421, 127876.	6.6	23
11228	Modeling Molecules under Pressure with Gaussian Potentials. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 583-597.	2.3	17
11229	Rotational spectrum and internal dynamics of the hydrogen-bonded pyrrole-pyridine aromatic pair. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 249, 119320.	2.0	1
11230	Inhibition of Urease, a Ni-Enzyme: The Reactivity of a Key Thiol With Mono- and Di-Substituted Catechols Elucidated by Kinetic, Structural, and Theoretical Studies. <i>Angewandte Chemie</i> , 2021, 133, 6094-6100.	1.6	3
11231	Adsorption of l-selenomethionine and l-selenocystine on the surface of silver nanoparticles: A spectroscopic study. <i>Nano Select</i> , 2021, 2, 47-60.	1.9	4
11232	Insight into the X-ray absorption spectra of Cu-porphyrazines from electronic structure theory. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26515.	1.0	3
11233	Adsorption studies of nucleobases on μ -arsenene nanosheet based on first-principles research. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 103, 107827.	1.3	16
11234	Macromolecular engineering in functional polymers via "click chemistry"™ using triazolinedione derivatives. <i>Progress in Polymer Science</i> , 2021, 113, 101343.	11.8	21
11235	Comprehensive Benchmark Study on the Calculation of ²⁹ Si NMR Chemical Shifts. <i>Inorganic Chemistry</i> , 2021, 60, 272-285.	1.9	14

#	ARTICLE	IF	CITATIONS
11236	Interplay of weak noncovalent interactions in alkoxybenzylidene derivatives of benzohydrazide and acetohydrazide: a combined experimental and theoretical investigation and lipoxygenase inhibition (LOX) studies. <i>CrystEngComm</i> , 2021, 23, 955-971.	1.3	9
11237	Coumarin-based Dye-sensitized solar cells (DSSCs): DFT and TD-DFT study of the spacer influence on photovoltaic properties. <i>Research on Chemical Intermediates</i> , 2021, 47, 875-893.	1.3	14
11238	Synthesis, crystal structure, Hirshfeld surface, DFT calculations, Z-scan and nonlinear optical studies of novel fluorinated hexahydropyrimidine. <i>Journal of Molecular Structure</i> , 2021, 1228, 129484.	1.8	15
11239	Oxidation of pentan-2-ol. Part I: Theoretical investigation on the decomposition and isomerization reactions of pentan-2-ol radicals. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 823-832.	2.4	7
11240	Novel Cu ²⁺ and Zn ²⁺ nanocomplexes drug based on hydrazone ligand bearings chromone and triazine moieties: Structural, spectral, DFT, molecular docking and cytotoxic studies. <i>Journal of Molecular Structure</i> , 2021, 1225, 129158.	1.8	24
11241	Stacking interactions in cavity-containing molecular structures built from acylphloroglucinols: a computational study. <i>Molecular Physics</i> , 2021, 119, e1800852.	0.8	2
11242	Can density functional theory (DFT) with highly fluxional shapeshifting molecules?. <i>Chemical Physics</i> , 2021, 540, 111013.	0.9	15
11243	Physical-chemical studies on putrescine (butane-1,4-diamine) and its solutions: Experimental and computational investigations. <i>Journal of Molecular Liquids</i> , 2021, 322, 114568.	2.3	0
11244	A study on the interaction of Nile blue with Uracils: A spectroscopic and computational approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 119011.	2.0	5
11245	A combined molecular dynamic simulation, DFT calculations, and experimental study of the Eriochrome Black T dye adsorption onto chitosan in aqueous solutions. <i>International Journal of Biological Macromolecules</i> , 2021, 166, 707-721.	3.6	54
11246	From a 1,2-azaborinine to large BN-PAHs via electrophilic cyclization: synthesis, characterization and promising optical properties. <i>Organic Chemistry Frontiers</i> , 2021, 8, 10-17.	2.3	14
11247	Electronic and Magnetic Properties of Transition Metal Doped ScN for Spintronics Applications. <i>Physica Status Solidi (B): Basic Research</i> , 2021, 258, 2000241.	0.7	1
11248	Reaction model and thermodynamic properties between sulfur-containing active groups and oxygen during coal self-heating. <i>Canadian Journal of Chemistry</i> , 2021, 99, 31-42.	0.6	4
11249	Mechanistic examination of C-H tyrosyl bond cleavage: Spectroscopic investigation of the generation of glyxyl radical cations from tyrosyl (glycyl/alanyl)tryptophan. <i>Journal of Mass Spectrometry</i> , 2021, 56, e4630.	0.7	1
11250	Insights into LiAlH ₄ Catalyzed Imine Hydrogenation. <i>Chemistry - A European Journal</i> , 2021, 27, 401-411.	1.7	24
11251	Density functional theoretical tailoring of electronic effect through various substituents on calix[4]arene-crown for efficient Cs ⁺ ion encapsulation and extraction. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26436.	1.0	1
11252	1D Coordination of Conjugated Polymers with Distinct Structures Defined by the Choice of the Transition Metal: Towards a New Class of Antiaromatic Macrocycles. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 439-445.	7.2	23
11253	1D Coordination of Conjugated Polymers with Distinct Structures Defined by the Choice of the Transition Metal: Towards a New Class of Antiaromatic Macrocycles. <i>Angewandte Chemie</i> , 2021, 133, 443-449.	1.6	0

#	ARTICLE	IF	CITATIONS
11254	Why Soot is not Alike Soot: A Molecular/Nanostructural Approach to Low Temperature Soot Oxidation. <i>Flow, Turbulence and Combustion</i> , 2021, 106, 295-329.	1.4	14
11255	Synthesis, spectrophotometric, voltammetric, and density functional theory studies of tetrahydro[3,2 <i>b</i>]indolocarbazoles for sensing small molecules. <i>Journal of Heterocyclic Chemistry</i> , 2021, 58, 127-136.	1.4	1
11256	Influence of Aryl Substituents on the Alignment of Ligands in the Dirhodium Tetrakis(1,2,2-triarylcyclopropane-carboxylate) Catalysts. <i>ChemCatChem</i> , 2021, 13, 174-179.	1.8	8
11257	Improved photovoltaic performance of phosphonic acid-based sensitized solar cells via an electron-withdrawing moiety: A density of functional theory study. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26431.	1.0	5
11258	Dinuclear Complex of Cu(II) Containing Chloride and Methoxide as Bridging-Ligands: A New Crystal Structure and DFT Calculations. <i>Journal of Chemical Crystallography</i> , 2021, 51, 1-8.	0.5	0
11259	Observation of quantum signature in rivastigmine chemical bond break-up and quantum energetics, spectral studies of anti-Alzheimer inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 118-128.	2.0	1
11260	How Do Ionic Liquids "Fold" Ionenenes? Computational and Experimental Analysis of Imidazolium Polymers Based on Ether and Alkyl Chain Variations Dissolved in an Ionic Liquid. <i>Macromolecules</i> , 2021, 54, 1611-1622.	2.2	4
11261	Effect of Polymerization on the Charge-Transfer Mechanism in the One (Two)-Photon Absorption Process of D-A-Type Triphenylamine Derivatives. <i>Journal of Physical Chemistry A</i> , 2021, 125, 777-794.	1.1	11
11262	Unimolecular Reactions Following Indoor and Outdoor Limonene Ozonolysis. <i>Journal of Physical Chemistry A</i> , 2021, 125, 669-680.	1.1	26
11263	Benchmarking dispersion-corrected DFT methods for the evaluation of materials with anisotropic properties: structural, electronic, dielectric, optical and vibrational analysis of calcite (CaCO ₃ , space group <i>R</i> _{3c}). <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18899-18907.	1.3	16
11264	Regioisomeric BODIPY derivatives: second-order nonlinear optical properties under an external electric field. <i>New Journal of Chemistry</i> , 2021, 45, 4335-4339.	1.4	1
11265	Metal-carbon bonding in perfluoroethylene and perfluorobenzene transition metal complexes. Some underappreciated <i>f</i> - and <i>l</i> f-acceptor components. , 2021, , 343-364.		0
11266	Mechanistic insights into the C-H activation of methane mediated by the unsupported and silica-supported VO ₂ OH and CrOOH: a DFT study. <i>RSC Advances</i> , 2021, 11, 11295-11303.	1.7	3
11267	Comparative Analysis of DFT+U, ACBN0, and Hybrid Functionals on the Spin Density of YTiO ₃ and SrRuO ₃ . <i>Applied Sciences (Switzerland)</i> , 2021, 11, 616.	1.3	1
11269	Synthesis and studies of covalently linked pyrrolyl bridged fluorescent dimers. <i>Journal of Porphyrins and Phthalocyanines</i> , 2021, 25, 418-427.	0.4	0
11270	Quantum computational investigations and molecular docking studies on amentoflavone. <i>Heliyon</i> , 2021, 7, e06079.	1.4	22
11271	Polythiophene derivatives as chemical sensors: a DFT study on the influence of side groups. <i>Journal of Molecular Modeling</i> , 2021, 27, 17.	0.8	11
11272	Magnetically induced ring currents in naphthalene-fused heteroporphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16629-16634.	1.3	2

#	ARTICLE	IF	CITATIONS
11273	CuAAC Mediated Synthesis of 2- <i>H</i> BT Linked Bioactive 1,2,3-Triazole Hybrids: Investigations through Fluorescence, DNA Binding, Molecular Docking, ADME Predictions and DFT Study. <i>ChemistrySelect</i> , 2021, 6, 685-694.	0.7	14
11274	Computational techniques for characterisation of electrically conductive MOFs: quantum calculations and machine learning approaches. <i>Journal of Materials Chemistry C</i> , 2021, 9, 13584-13599.	2.7	14
11275	Conformational energies and equilibria of cyclic dinucleotides in vacuo and in solution: computational chemistry vs. NMR experiments. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7280-7294.	1.3	5
11276	Self-assembly of the cationic surfactant <i>n</i> -hexadecyl-trimethylammonium chloride in methyltrimethoxysilane aqueous solution: classical and reactive molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14486-14495.	1.3	7
11277	Computational Investigation on the Thermodynamics of H ₂ CO + NH ₂ → NH ₂ CHO + H on Interstellar Water Ice Surfaces. <i>Lecture Notes in Computer Science</i> , 2021, , 658-666.	1.0	1
11278	A simplified charge projection scheme for long-range electrostatics in <i>ab initio</i> QM/MM calculations. <i>Journal of Chemical Physics</i> , 2021, 154, 024115.	1.2	18
11279	Electrocatalytic nitrate reduction with Co-based catalysts: comparison of DIM, TIM and cyclam ligands. <i>Dalton Transactions</i> , 2021, 50, 12324-12331.	1.6	8
11280	Radical cations and dications of bis[1]benzothieno[1,4]thiazine isomers. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5744-5755.	2.3	2
11281	Fused Thiazine Tethered Metal-Free Dyes for Dye Sensitized Solar Cells: A Computational Investigation. <i>Asian Journal of Chemistry</i> , 2021, 33, 2373-2378.	0.1	0
11282	Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) as a Simple yet Accurate Method for Diradicals and Diradicaloids. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 848-859.	2.3	29
11283	Equivalent Loading of Directed Arenes in Pd(II)-Catalyzed Oxidative Cross-Coupling of Aryl C-H Bonds at Room Temperature. <i>Journal of Organic Chemistry</i> , 2021, 86, 2714-2733.	1.7	7
11284	Revealing structural peculiarities of homopurine GA repetition stuck by i-motif clip. <i>Nucleic Acids Research</i> , 2021, 49, 11425-11437.	6.5	3
11285	Localized and Delocalized States of a Diamine Cation: Resolution of a Controversy. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1250-1255.	2.1	3
11286	Molecular Mechanism for the Self-Supported Synthesis of Graphitic Carbon Nitride from Urea Pyrolysis. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1396-1406.	2.1	20
11287	Dissociative Photoionization of Methyl Vinyl Ketone ~ Thermochemical Anchors and a Drifting Methyl Group. <i>Journal of Physical Chemistry A</i> , 2021, 125, 848-856.	1.1	3
11288	Method Optimisation in Hydrophilic-Interaction Liquid Chromatography by Design of Experiments Combined with Quantitative Structure-Retention Relationships. <i>Australian Journal of Chemistry</i> , 2021, 74, 778-786.	0.5	4
11289	An electron rich indaceno [2,1- <i>b</i> :6,5- <i>b'</i>] dithiophene derivative as a high intramolecular charge transfer material in dye sensitized solar cells. <i>New Journal of Chemistry</i> , 2021, 45, 2734-2741.	1.4	4
11290	Theoretical study on the electronic and optical properties of strain-tuned CsPb(1-xBrx) ₃ and CsSn(1-xBrx) ₃ . <i>Chemical Physics Letters</i> , 2021, 763, 138219.	1.2	5

#	ARTICLE	IF	CITATIONS
11291	Studies on chemoselective synthesis of 1,4- and 1,2-dihydropyridine derivatives by a Hantzsch-like reaction: a combined experimental and DFT study. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 3882-3892.	1.5	6
11292	<i>Ab initio</i> rate coefficients for reactions of 2,5-dimethylhexyl isomers with O ₂ : temperature- and pressure-dependent branching ratios. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6225-6240.	1.3	3
11293	Benzobisthiadiazole-based high-spin donor-acceptor conjugated polymers with localized spin distribution. <i>Materials Advances</i> , 2021, 2, 2943-2955.	2.6	10
11294	A theoretical study on solvatochromic asymmetric thiazolothiazole (TTz) dyes using dielectric-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21078-21086.	1.3	4
11295	Study of the structural and optoelectronic properties of dye solar cells based on phosphonic acid anchoring by DFT functionals. <i>New Journal of Chemistry</i> , 2021, 45, 2723-2733.	1.4	12
11296	A Quantum Chemistry View on Two Archetypical Paramagnetic Pentacoordinate Nickel(II) Complexes Offers a Fresh Look on Their NMR Spectra. <i>Inorganic Chemistry</i> , 2021, 60, 2068-2075.	1.9	18
11297	Exploration of CH ₃ F & CF ₃ H mediated supramolecular arrangements into fluorinated terphenyls and theoretical prediction of their third-order nonlinear optical response. <i>RSC Advances</i> , 2021, 11, 7766-7778.	1.7	36
11298	Reactivity of a T-shaped cobalt(<i>scp</i>) pincer-complex. <i>Dalton Transactions</i> , 2021, 50, 6802-6810.	1.6	3
11299	Calculated oxidation potentials predict reactivity in Baeyer-Mills reactions. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 7575-7580.	1.5	8
11300	DFT studies on Ni-catalyzed intermolecular cycloaddition of diynes with methyleneaziridines. <i>Dalton Transactions</i> , 2021, 50, 12308-12315.	1.6	1
11301	Unusual rearrangement-remercuration reactions of allylic silanols. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5361-5368.	2.3	8
11302	Polymorphism of chitosan-based networks stabilized by phytate investigated by molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22601-22612.	1.3	4
11303	The Fascinating Chemistry of Mesoionic 4-Trifluoroacetyl-1,3-oxazolium-5-olates and Related Compounds. <i>Heterocycles</i> , 2021, 102, 1643.	0.4	2
11304	Influence of solution chemistry on the solubility, crystallisability and nucleation behaviour of eicosane in toluene-acetone mixed-solvents. <i>CrystEngComm</i> , 2021, 23, 3109-3125.	1.3	7
11305	Computational exploration of heterometal substitution into the decaniobate framework, [Nb ₁₀ O ₂₈] ⁶⁺ . <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10402-10408.	1.3	0
11306	Structures and hydrogen bonding of 1,7-dioxaspiro[5.5]undecane and its hydrates. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19289-19296.	1.3	1
11307	Reduced-dimensional surface hopping with offline-online computations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19547-19557.	1.3	2
11308	Isoquinoline-based Eu(<i>scp</i>) luminescent probes for citrate sensing in complex matrix. <i>Dalton Transactions</i> , 2021, 50, 4700-4712.	1.6	8

#	ARTICLE	IF	CITATIONS
11309	Theoretical calculation of newly synthesized tetrazolopyrimidine derivatives as a potential corrosion inhibitor. <i>Journal of the Serbian Chemical Society</i> , 2022, 87, 575-587.	0.4	1
11310	High coordination number actinide-noble gas complexes; a computational study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4167-4177.	1.3	3
11311	Phthalimide conjugation turns the AIE-active tetraphenylethylene unit non-emissive: its use in turn-on sensing of hydrazine in solution and the solid- and vapour-phase. <i>RSC Advances</i> , 2021, 11, 21269-21278.	1.7	11
11312	Theoretical investigation of polymorph- and coformer-dependent photoluminescence in molecular crystals. <i>CrystEngComm</i> , 2021, 23, 4264-4271.	1.3	9
11313	Adducts of Hydroxybenzenes with Explicit Acetonitrile Molecules. <i>Progress in Theoretical Chemistry and Physics</i> , 2021, , 267-287.	0.2	0
11314	Gem-dimethyl peptide nucleic acid (\hat{I}^2/\hat{I}^3 -PNA) monomers: synthesis and the role of \hat{I}^3 -substituents in preferential stabilisation of \hat{Z} / \hat{E} -rotamers. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 6534-6545.	1.5	5
11315	Hydrogen evolution by polymer photocatalysts; a possible photocatalytic cycle. <i>Sustainable Energy and Fuels</i> , 2021, 5, 2622-2632.	2.5	10
11316	Revisiting activity of some glucocorticoids as a potential inhibitor of SARS-CoV-2 main protease: theoretical study. <i>RSC Advances</i> , 2021, 11, 10027-10042.	1.7	56
11317	The mystery of sub-picosecond charge transfer following irradiation of hydrated uridine monophosphate. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21148-21162.	1.3	10
11318	Doubly fused fluorene embedded heterosapphyrins. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3059-3068.	2.3	8
11319	1,2,3-Triazole framework: a strategic structure for $\hat{H}\hat{X}$ hydrogen bonding and practical design of an effective Pd-catalyst for carbonylation and carbon-carbon bond formation. <i>RSC Advances</i> , 2021, 11, 20812-20823.	1.7	7
11320	Hydrogenation of Cyclic 1,3-Diones to Their 1,3-Diols Using Heterogeneous Catalysts: Toward a Facile, Robust, Scalable, and Potentially Bio-Based Route. <i>ACS Omega</i> , 2021, 6, 4313-4328.	1.6	4
11321	An enantiomeric pair of alkaline-earth metal based coordination polymers showing room temperature phosphorescence and circularly polarized luminescence. <i>Journal of Materials Chemistry C</i> , 2021, 9, 5544-5553.	2.7	10
11322	The structural manipulation of a series of Ni_4 defective dicubanes: Synthesis, X-ray Structures, Magnetic and Computational analyses. <i>Dalton Transactions</i> , 2021, 50, 5318-5326.	1.6	5
11323	Copper(II) complexes of 2-methyl-8-hydroxyquinoline and tri/diimine co-ligand: DFT calculations, DNA and BSA binding, DNA cleavage, cytotoxicity and induction of apoptosis. <i>New Journal of Chemistry</i> , 2021, 45, 7578-7593.	1.4	5
11324	On the structure and reactivity of Pt_nCu_n ($n = 1-7$) alloy clusters. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7233-7239.	1.3	10
11325	Between T and Y: Asymmetry in the Interaction of LAu(I) with Bipy and \hat{I}^2 -diiminate-like Ligands. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 314-320.	1.0	2
11326	How many shades of grey? On the proximity of density functional approximation to ab initio method via calculations of electric multipole moments. <i>Journal of Physics: Conference Series</i> , 2021, 1730, 012126.	0.3	0

#	ARTICLE	IF	CITATIONS
11327	Structural and electronic properties of TiO ₂ from first principles calculations. , 2021, , 67-85.		2
11328	Interplay between non-covalent interactions in 1D supramolecular polymers based on 1,4-bis(iodoethynyl)benzene. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 3531-3542.	1.3	3
11329	DBU and TU synergistically induced ring-opening polymerization of phosphate esters: a mechanism study. <i>New Journal of Chemistry</i> , 2021, 45, 1953-1958.	1.4	2
11330	Mechanism of Pd-catalysed C(sp ³)â€“H arylation of thioethers with Ag(<i>scp</i>) additives. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 6766-6770.	1.5	3
11332	Donor acceptor fluorophores: synthesis, optical properties, TD-DFT and cytotoxicity studies. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 1835-1846.	1.5	12
11333	Efficient and low-scaling linear-response time-dependent density functional theory implementation for core-level spectroscopy of large and periodic systems. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4736-4746.	1.3	14
11334	Design and DFT study of nitrogen-rich donor systems for improved photovoltaic performance in dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2021, 45, 11585-11595.	1.4	16
11335	Quantitative Comparison of Experimental and Computed IR-Spectra Extracted from Ab Initio Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 985-995.	2.3	9
11336	High-Resolution Rotational Spectroscopy and Interstellar Search for Isopropyl Isothiocyanate. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 33-39.	1.2	4
11337	High-Rate Long Cycle-Life Li-Air Battery Aided by Bifunctional InX ₃ (X = I and Br) Redox Mediators. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 4915-4922.	4.0	17
11338	Mechanism of nickel-catalyzed direct carbonyl-Heck coupling reaction: the crucial role of second-sphere interactions. <i>Dalton Transactions</i> , 2021, 50, 2654-2662.	1.6	10
11339	Insights into the structure and ionic transport in â€“water-in-bisaltâ€“™ electrolytes for lithium-ion batteries. <i>Materials Advances</i> , 2021, 2, 7691-7700.	2.6	4
11340	Blue LED-Mediated Nâ€“H Insertion of Indoles into Aryldiazoesters at Room Temperature in Batch and Flow: Reaction Kinetics, Density Functional Theory, and Mechanistic Study. <i>Journal of Organic Chemistry</i> , 2021, 86, 2522-2533.	1.7	25
11341	Estimation of the relative contributions to the electronic energy transfer rates based on FÃ¶rster theory: The case of C-phycocyanin chromophores. <i>Biophysics and Physicobiology</i> , 2021, 18, 196-214.	0.5	3
11342	Charge Transfer Excitation and Asymmetric Energy Transfer at the Interface of Pentaceneâ€“Perfluoropentacene Heterostacks. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 5284-5292.	4.0	5
11343	A Computational Analysis of the Reaction of Atomic Oxygen O(\$^3\$P) with Acrylonitrile. <i>Lecture Notes in Computer Science</i> , 2021, , 339-350.	1.0	0
11344	Excitonic and charge transfer interactions in tetracene stacked and T-shaped dimers. <i>Journal of Chemical Physics</i> , 2021, 154, 044306.	1.2	11
11345	Replacing hybrid density functional theory: motivation and recent advances. <i>Chemical Society Reviews</i> , 2021, 50, 8470-8495.	18.7	80

#	ARTICLE	IF	CITATIONS
11346	The necessity of periodic boundary conditions for the accurate calculation of crystalline terahertz spectra. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20038-20051.	1.3	19
11347	One-pot hydrodeoxygenation of bioderived furans into octane at low temperatures <i>via</i> an octanediol route. <i>Green Chemistry</i> , 2021, 23, 4741-4752.	4.6	10
11348	Halogenation affects driving forces, reorganization energies and "rocking" motions in strained [Fe(tpy) ₂] ²⁺ complexes. <i>Dalton Transactions</i> , 2021, 50, 14566-14575.	1.6	6
11349	Alkoxy functionalized benzothiadiazole based donor-acceptor conjugated copolymers for organic field-effect transistors. <i>Journal of Materials Chemistry C</i> , 2021, 9, 5113-5123.	2.7	22
11350	Origins of ligand-controlled diastereoselectivity in dirhodium-catalysed direct amination of aliphatic C(sp ³)-H bonds. <i>Catalysis Science and Technology</i> , 2021, 11, 6960-6964.	2.1	2
11351	Computational Exploration of Intramolecular Sn/N Frustrated Lewis Pairs for Hydrogen Activation and Catalytic Hydrogenation. <i>Organometallics</i> , 2021, 40, 194-202.	1.1	8
11352	Predicting the structure and NMR coupling constant ¹²⁹ Xe- ¹⁹ F of XeF ₆ using quantum mechanics methods. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7240-7246.	1.3	2
11353	A photoelectron imaging study of the deprotonated GFP chromophore anion and RNA fluorescent tags. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19911-19922.	1.3	3
11354	Assessment of the performance of DFT functionals in the fulfillment of off-diagonal hypervirial relationships. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15268-15274.	1.3	13
11355	Crystal Packing Studies, Thermal Properties and Hirshfeld Surface Analysis in the Zn(II) Complex of 3-Aminopyridine with Thiocyanate as Co-Ligand. <i>Open Journal of Inorganic Chemistry</i> , 2021, 11, 63-84.	0.7	2
11356	¹³ C NMR chemical shift assignments of nitrated benzo[a]pyrenes based on two-dimensional techniques and DFT/GIAO calculations. <i>Results in Chemistry</i> , 2021, 3, 100099.	0.9	6
11357	Experimental and Theoretical Studies on Effects of Structural Modification of Tin Nanoclusters for Third-Order Nonlinear Optical Properties. <i>Inorganic Chemistry</i> , 2021, 60, 1885-1892.	1.9	21
11358	Optical Properties of the Atomically Precise C ₄ Core [Au ₉ (PPh ₃) ₈] ³⁺ Cluster Probed by Transient Absorption Spectroscopy and Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2033-2044.	1.5	8
11359	Molecular Simulation Study of Gold Clusters for Transporting of Thioguanine Anticancer Drug in Aqueous Solution. <i>Journal of Cluster Science</i> , 2022, 33, 135-143.	1.7	6
11360	Chromous carbonates containing a square-grid layer of {Cr ₂ (CO ₃) ₄ } _n ⁴ⁿ⁺ based on a dichromium(<i>ii</i>) paddlewheel core. <i>Dalton Transactions</i> , 2021, 50, 2387-2392.	1.6	3
11361	Enantiomeric Separation of Semiconducting Single-Walled Carbon Nanotubes by Acid Cleavable Chiral Polyfluorene. <i>ACS Nano</i> , 2021, 15, 4699-4709.	7.3	25
11362	QM/MM study of the binding of H ₂ to MoCu CO dehydrogenase: development and applications of improved H ₂ van der Waals parameters. <i>Journal of Molecular Modeling</i> , 2021, 27, 68.	0.8	4
11363	Zeolite catalyzed hydroarylation of alkenes with aromatic amines under organic ligand-free conditions. <i>Journal of Catalysis</i> , 2021, 394, 18-29.	3.1	6

#	ARTICLE	IF	CITATIONS
11364	Pyochelin Biosynthetic Metabolites Bind Iron and Promote Growth in <i>Pseudomonads</i> Demonstrating Siderophore-like Activity. <i>ACS Infectious Diseases</i> , 2021, 7, 544-551.	1.8	16
11365	A Substituent-Directed Strategy for the Selective Synthesis of Hexoses: An Expedient Route to Dose. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 1575-1584.	1.2	4
11366	Autocatalytic photoredox Chan-Lam coupling of free diaryl sulfoximines with arylboronic acids. <i>Nature Communications</i> , 2021, 12, 932.	5.8	34
11367	Theoretical Studies of Rare-Earth-Catalyzed [3 + 2] Annulation of Aromatic Aldimine with Styrene: Mechanism and Origin of Diastereoselectivity. <i>Journal of Organic Chemistry</i> , 2021, 86, 4236-4244.	1.7	16
11368	Non-Covalent Interactions Atlas Benchmark Data Sets 3: Repulsive Contacts. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1548-1561.	2.3	42
11369	Epoxy Functional Composites Based on Lanthanide Metal-Organic Frameworks for Luminescent Polymer Materials. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 7625-7634.	4.0	26
11370	What Types of Chemical Problems Benefit from Density-Corrected DFT? A Probe Using an Extensive and Chemically Diverse Test Suite. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1368-1379.	2.3	45
11371	N,N- and N,O-membered Ring pericyclic Annulation in Naphthalene. Is it a Heteroring or merely a pericyclic Heterobridge?. <i>ChemistrySelect</i> , 2021, 6, 951-961.	0.7	2
11372	Excited-State Properties and Relaxation Pathways of Selenium-Substituted Guanine Nucleobase in Aqueous Solution and DNA Duplex. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1778-1789.	1.2	18
11373	Degradation of Organophosphates Promoted by 1,2,4-Triazole Anion: Exploring Scaffolds for Efficient Catalytic Systems. <i>Journal of Organic Chemistry</i> , 2021, 86, 4027-4034.	1.7	7
11374	Atomic chain of carbon atoms: Smallest negative differential resistance device. <i>Journal of Physics: Conference Series</i> , 2021, 1797, 012047.	0.3	0
11375	Magnetic properties and electronic structures of ultrathin SrMnO ₃ /LaAlO ₃ (001) heterostructure. <i>Physica B: Condensed Matter</i> , 2021, 603, 412790.	1.3	1
11376	Oxidative detoxification of nerve agent VX simulant by polyoxoniobate: Experimental and theoretical insights. <i>Journal of Catalysis</i> , 2021, 394, 83-93.	3.1	6
11377	Single-Point Hessian Calculations for Improved Vibrational Frequencies and Rigid-Rotor-Harmonic-Oscillator Thermodynamics. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1701-1714.	2.3	49
11378	XABOOM: An X-ray Absorption Benchmark of Organic Molecules Based on Carbon, Nitrogen, and Oxygen 1s $\pi^* \leftarrow \pi$ Transitions. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1618-1637.	2.3	37
11379	How Lewis Acids Catalyze Ring-Openings of Cyclohexene Oxide. <i>Journal of Organic Chemistry</i> , 2021, 86, 3565-3573.	1.7	28
11380	Demystifying Chronic Kidney Disease of Unknown Etiology (CKDu): Computational Interaction Analysis of Pesticides and Metabolites with Vital Renal Enzymes. <i>Biomolecules</i> , 2021, 11, 261.	1.8	5
11381	Kinetics of the Thermal Decomposition of Ethylsilane: Shock-Tube and Modeling Study. <i>Energy & Fuels</i> , 2021, 35, 3266-3282.	2.5	5

#	ARTICLE	IF	CITATIONS
11382	A density functional theory (DFT) study of the doping effect on 4-[2-(2-N, N-dihydroxy amino thiophene) vinyl] benzenamine. <i>SN Applied Sciences</i> , 2021, 3, 1.	1.5	4
11383	Effect of Nanopore Geometry in the Conformation and Vibrational Dynamics of a Highly Confined Molecular Glass. <i>Nano Letters</i> , 2021, 21, 1778-1784.	4.5	5
11384	Electron Density-based Estimation of Diradical Character: An Easy Scheme for DFT/Plane-wave Calculations. <i>Chemistry Letters</i> , 2021, 50, 392-396.	0.7	6
11385	Redox behavior, spectroscopic investigations, theoretical interpretation and biological effectiveness of some novel prepared bis-azomethine derivatives and their copper(II) complexes. <i>Journal of Coordination Chemistry</i> , 2021, 74, 779-803.	0.8	2
11386	Switching Site Reactivity in Hydrogenase Model Systems by Introducing a Pendant Amine Ligand. <i>ACS Omega</i> , 2021, 6, 4192-4203.	1.6	6
11387	Effect of varying the TD-Ic-DFTB range-separation parameter on charge and energy transfer in a model pentacene/buckminsterfullerene heterojunction. <i>Journal of Chemical Physics</i> , 2021, 154, 054102.	1.2	9
11388	Tuning the H-Atom Transfer Reactivity of Iron(IV)-Oxo Complexes as Probed by Infrared Photodissociation Spectroscopy. <i>Angewandte Chemie</i> , 2021, 133, 7202-7207.	1.6	4
11389	Tuning the H-Atom Transfer Reactivity of Iron(IV)-Oxo Complexes as Probed by Infrared Photodissociation Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 7126-7131.	7.2	17
11391	Atomic structural and electronic bandstructure calculations for borophene. <i>Materials Research Express</i> , 2021, 8, 026301.	0.8	5
11392	Phenanthroline-Catalyzed Stereoselective Formation of \pm -1,2- <i>cis</i> -2-Deoxy-2-Fluoro Glycosides. <i>ACS Catalysis</i> , 2021, 11, 2108-2120.	5.5	12
11393	Do Secondary Electrostatic Interactions Influence Multiple Dihydrogen Bonds? AA ⁺ DD Array on an Amine-Borane Aza-Coronand: Theoretical Studies and Synthesis. <i>ChemPhysChem</i> , 2021, 22, 593-605.	1.0	9
11394	Density Functional Theory Investigation of Structure-Activity Relationship for Efficient Electrochemical CO ₂ Reduction on Defective SnSe ₂ Nanosheets. <i>ACS Applied Nano Materials</i> , 2021, 4, 2760-2767.	2.4	6
11395	Effect of AlEt ₂ Cl on the polymerization of isoprene using TiCl ₄ /MgCl ₂ type Ziegler-Natta catalyst: A DFT study. <i>Molecular Catalysis</i> , 2021, 502, 111399.	1.0	0
11396	Revisiting the OH + H ₂ → H ₂ O + H reaction at the molecular level: the plausible catalytic role of ice in its own reconstruction. <i>Astronomy and Astrophysics</i> , 2021, 646, A163.	2.1	4
11397	Tuning π -Acceptor/ σ -Donor Ratio of the 2-Isocyanoazulene Ligand: Non-Fluorinated Rival of Pentafluorophenyl Isocyanide and Trifluorovinyl Isocyanide Discovered. <i>Molecules</i> , 2021, 26, 981.	1.7	2
11398	In-situ photochemical synthesis and dielectric properties of nanocomposite thin films containing Au, Ag and MnO nanoparticles. <i>European Polymer Journal</i> , 2021, 144, 110238.	2.6	11
11399	Quantifying bond strengths via a Coulombic force model: application to the impact sensitivity of nitrobenzene, nitrogen-rich nitroazole, and non-aromatic nitramine molecules. <i>Journal of Molecular Modeling</i> , 2021, 27, 69.	0.8	6
11400	Modeling One- and Two-Photon Excitation of 4-(Hydroxymethyl)-4,5,8-trimethylpsoralen in Complex with DNA: Solving Electron Spill-Out Problems in Polarizable QM/MM Calculations. <i>Advanced Theory and Simulations</i> , 2021, 4, 2000294.	1.3	4

#	ARTICLE	IF	CITATIONS
11401	Efficient enumeration of bosonic configurations with applications to the calculation of non-radiative rates. <i>Journal of Chemical Physics</i> , 2021, 154, 084102.	1.2	5
11402	Can enhancement in tunnelling width influence the final spintronic feature of two-dimensional nanostructure of graphitic carbon nitride-(graphene)- graphitic carbon nitride?. <i>Journal of Physics: Conference Series</i> , 2021, 1797, 012046.	0.3	1
11403	Breaking the Controversy of the Electropolymerization of Pyrrole Mechanisms by the Effective Screening Medium Quantum Charged Model Interface. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1860-1869.	1.1	2
11404	Benchmarking Magnetizabilities with Recent Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1457-1468.	2.3	43
11405	First-Principles Investigations of Magnetic Anisotropy and Spin-Crossover Behavior of Fe(III)â€“TBP Complexes. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2197-2207.	1.1	10
11406	Understanding and Designing Tailor-Made Additives for Controlling Nucleation: Case Study of <i>p</i> -Aminobenzoic Acid Crystallizing from Ethanolic Solutions. <i>Crystal Growth and Design</i> , 2021, 21, 1946-1958.	1.4	22
11407	How Can We Predict Accurate Electrochromic Shifts for Biochromophores? A Case Study on the Photosynthetic Reaction Center. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1858-1873.	2.3	18
11408	Improving the Performance of Perovskite Solar Cells via a Novel Additive of <i>N</i> -Fluoroformamidinium Iodide with Electronâ€“Withdrawing Fluorine Group. <i>Advanced Functional Materials</i> , 2021, 31, 2010603.	7.8	37
11409	Computational modelling of potent Î²-secretase (BACE1) inhibitors towards Alzheimer's disease treatment. <i>Biophysical Chemistry</i> , 2021, 270, 106536.	1.5	14
11410	The bandgap regulation and optical properties of alloyed Cs ₂ NaSbX ₆ (X=Cl, Br, I) systems with first principle method. <i>Journal of Materials Research and Technology</i> , 2021, 11, 1645-1653.	2.6	10
11411	Ensemble generalized Kohnâ€“Sham theory: The good, the bad, and the ugly. <i>Journal of Chemical Physics</i> , 2021, 154, 094125.	1.2	12
11412	Photooxidation of Isoprene by Titanium Oxide Cluster Anions with Dimensions up to a Nanosize. <i>Journal of the American Chemical Society</i> , 2021, 143, 3951-3958.	6.6	15
11413	Non-Aufbau Spiro-Conjugated Quinoidal & Aromatic Charged Radicals. <i>Bulletin of the Chemical Society of Japan</i> , 2021, 94, 989-996.	2.0	8
11414	A Long Residence Time Enoyl-Reductase Inhibitor Explores an Extended Binding Region with Isoenzyme-Dependent Tautomer Adaptation and Differential Substrate-Binding Loop Closure. <i>ACS Infectious Diseases</i> , 2021, 7, 746-758.	1.8	4
11415	Axial Redox Tuning at a Tetragonal Cobalt Center. <i>Inorganic Chemistry</i> , 2021, 60, 5647-5659.	1.9	2
11416	DFT study of the interaction between carbon monoxide and Rh-Cu bimetallic nanoclusters. <i>Materials Today Communications</i> , 2021, 26, 102013.	0.9	5
11417	Localized electronic vacancy level and its effect on the properties of doped manganites. <i>Scientific Reports</i> , 2021, 11, 6706.	1.6	8
11418	Water Molecules Allow the Intramolecular Activation of the Thiamine Di-Phosphate Cofactor in Human Transketolase: Mechanistic Insights into a Famous Proposal. <i>ACS Catalysis</i> , 2021, 11, 4136-4145.	5.5	4

#	ARTICLE	IF	CITATIONS
11419	DFT analysis of the structures, dynamics and reactivity of [(Propargyl)Co ₂ (CO) ₅ (L)] ⁺ Z ⁻ . Journal of Organometallic Chemistry, 2021, 935, 121667.	0.8	0
11420	Effects of Fe doping on the visible light absorption and bandgap tuning of lead-free (CsSnCl ₃) and lead halide (CsPbCl ₃) perovskites for optoelectronic applications. AIP Advances, 2021, 11, .	0.6	20
11421	Combination Regimen of Amino-Noscapine and Docetaxel for Evaluation of Anticancer Activity. Analytical Chemistry Letters, 2021, 11, 215-229.	0.4	3
11422	A DFT study on stability and electronic structure of AlN nanotubes. Materials Today Communications, 2021, 26, 102118.	0.9	13
11423	Theoretical prediction of the host of Helium: (HSiO ₃ /2) _n (n ⁻ =4, 6, 8) POSS material. Materials Today Communications, 2021, 26, 101972.	0.9	0
11424	Hyperpolarized ¹³ C Magnetic Resonance Imaging of Fumarate Metabolism by Parahydrogen-induced Polarization: A Proof-of-Concept <i>in vivo</i> Study. ChemPhysChem, 2021, 22, 1.0 915-923.	1.0	22
11425	Do Docking Sites Persist Upon Fluorination? The Diadamantyl Ether-Aromatics Challenge for Rotational Spectroscopy and Theory. Chemistry - A European Journal, 2021, 27, 6198-6203.	1.7	10
11426	Confinement of the antitumoral drug cisplatin inside edge-functionalized carbon nanotubes and its release near lipid membrane. European Physical Journal D, 2021, 75, 1.	0.6	4
11427	Monte-Carlo Simulations of Soft Matter Using SIMONA: A Review of Recent Applications. Frontiers in Physics, 2021, 9, .	1.0	6
11428	First principle investigation of new metal-free organic dye molecular for DSSCs: effects of Ï-conjugated groups. Molecular Simulation, 0, , 1-7.	0.9	2
11429	Accelerate stochastic calculation of random-phase approximation correlation energy difference with an atom-based correlated sampling. Electronic Structure, 2021, 3, 014003.	1.0	0
11430	Polarons in materials. Nature Reviews Materials, 2021, 6, 560-586.	23.3	273
11431	Spin-Conserved and Spin-Flip Optical Excitations from the Bethe-Salpeter Equation Formalism. Journal of Chemical Theory and Computation, 2021, 17, 2852-2867.	2.3	15
11432	Gallium chloride phthalocyanines possessing 4-(trifluoromethoxy)phenoxy units: Synthesis, characterization, and photophysical investigations. Journal of the Chinese Chemical Society, 2021, 68, 1466-1477.	0.8	3
11433	The TDDFT Excitation Energies of the BODIPYs; The DFT and TDDFT Challenge Continues. Molecules, 2021, 26, 1780.	1.7	13
11434	Key Mechanistic Features of the Silver(I)-Mediated Deconstructive Fluorination of Cyclic Amines: Multistate Reactivity versus Single-Electron Transfer. Journal of the American Chemical Society, 2021, 143, 3889-3900.	6.6	20
11435	Molecular Conformation of Bent-Core Molecules Affected by Chiral Side Chains Dictates Polymorphism and Chirality in Organic Nano- and Microfilaments. ACS Nano, 2021, 15, 7249-7270.	7.3	16
11436	The role of the synthetic chromophore of GFP in generating polymorphism-dependent on/off photoluminescence. Dyes and Pigments, 2021, 187, 109119.	2.0	3

#	ARTICLE	IF	CITATIONS
11437	Optimization of Three State Conical Intersections by Adaptive Penalty Function Algorithm in Connection with the Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory Method (MRSF-TDDFT). <i>Journal of Physical Chemistry A</i> , 2021, 125, 1994-2006.	1.1	21
11438	Vibrationally Assisted Direct Intersystem Crossing between the Same Charge-Transfer States for Thermally Activated Delayed Fluorescence: Analysis by Marcus's Hush Theory Including Reorganization Energy. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2696-2706.	1.2	35
11439	Anionic Thia-Fries Rearrangement at Ferrocene: A Computational and Experimental Study. <i>Helvetica Chimica Acta</i> , 2021, 104, e2100025.	1.0	3
11440	Screening Nanographene-Mediated Inter(Porphyrin) Communication to Optimize Inter(Porphyrin-Fullerene) Forces. <i>Advanced Energy Materials</i> , 2021, 11, 2100158.	10.2	9
11441	Electronic, vibrational and optical properties of two-electron atoms and ions trapped in small fullerene-like cages. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2021, 54, 065101.	0.6	0
11442	Application of Optimization Algorithms in Clusters. <i>Frontiers in Chemistry</i> , 2021, 9, 637286.	1.8	6
11443	Gold-catalyzed ketene dual functionalization and mechanistic insights: divergent synthesis of indenones and benzo[d]oxepines. <i>Science China Chemistry</i> , 2021, 64, 778-787.	4.2	23
11444	Revisiting Activity of Some Nocodazole Analogues as a Potential Anticancer Drugs Using Molecular Docking and DFT Calculations. <i>Frontiers in Chemistry</i> , 2021, 9, 628398.	1.8	66
11445	Adsorption of Ag on M-doped graphene: First principle calculations. <i>International Journal of Minerals, Metallurgy and Materials</i> , 2021, 28, 487-494.	2.4	14
11446	Ligand Architecture Perturbation Influences the Reactivity of Nonheme Iron(V)-Oxo Tetraamido Macrocyclic Ligand Complexes: A Combined Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2021, 60, 4058-4067.	1.9	7
11447	Triggering Electron Transfer in Co(I) Dimers: Computational Evidences for a Reversible Disproportionation Mechanism. <i>ChemPhysChem</i> , 2021, 22, 788-795.	1.0	1
11448	Controlled post-polymerization modification through modulation of repeating unit reactivity: Proof of concept discussed using linear polyethylenimine example. <i>Polymer</i> , 2021, 217, 123452.	1.8	3
11449	Density Functional Theory Modeling of Reactions of Addition of H ₂ Molecules to Magnesium Clusters Mg ₁₇ M Doped with Atoms M of Transition 3d Elements. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2308-2315.	1.1	11
11450	Explaining and Fixing DFT Failures for Torsional Barriers. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2796-2804.	2.1	23
11451	Analytical derivatives of the individual state energies in ensemble density functional theory. II. Implementation on graphical processing units (GPUs). <i>Journal of Chemical Physics</i> , 2021, 154, 104108.	1.2	8
11452	A dual-response naphthalene-armed calix[4]arene based fluorescence receptor for Zr(IV) and Fe(II) via Ligand to metal charge transfer. <i>Sensors and Actuators B: Chemical</i> , 2021, 331, 129417.	4.0	15
11453	Bay-Substitution Effect of Perylene Diimides on Supramolecular Chirality and Optoelectronic Properties of Their Self-Assembled Nanostructures. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 12278-12285.	4.0	16
11454	Extraction of uranium from sulfuric acid media using amino-diamide extractants. <i>Hydrometallurgy</i> , 2021, 200, 105550.	1.8	8

#	ARTICLE	IF	CITATIONS
11455	Antinörodejeneratif 5-sabit 2,4-tiyazolidindion Tervlerinin Kuantum Kimyasal ncelemesi. Erzincan niversitesi Fen Bilimleri Enstitüsü Dergisi, 0, , .	0.1	0
11456	Study of bandgap tuning of In _{1-x} GaxY (Y = N, P) alloys for optoelectronic applications: abinitio calculations. Chinese Physics B, 0, , .	0.7	1
11457	A theoretical and experimental study of phosphate ester inhibitors for AISI 1018 in carbon dioxide-saturated 3.5%wt% NaCl solution. Materials and Corrosion - Werkstoffe Und Korrosion, 2021, 72, 1417-1432.	0.8	2
11458	Ni/Cu-catalyzed silylation of allylic alcohol: Theoretical studies on the mechanisms, regioselectivity, and role of ligand. Molecular Catalysis, 2021, 504, 111456.	1.0	1
11459	Molecular Mechanism of Thermal Dry Etching of Iron in a Two-Step Atomic Layer Etching Process: Chlorination Followed by Exposure to Acetylacetone. Journal of Physical Chemistry C, 2021, 125, 7142-7154.	1.5	10
11460	Signatures of Conical Intersection Dynamics in the Time-Resolved Photoelectron Spectrum of Furan: Theoretical Modeling with an Ensemble Density Functional Theory Method. International Journal of Molecular Sciences, 2021, 22, 4276.	1.8	4
11461	The second-order nonlinear optical property of hydrazones-based photochromic complexes: A DFT study. Journal of Molecular Liquids, 2021, 327, 114882.	2.3	13
11462	A zero dimensional hybrid organic- inorganic perovskite CuCl ₄ based: Synthesis, crystal structure, vibrational, optical properties, DFT and TDFT calculations, dielectric properties and biological activity. Journal of Molecular Structure, 2021, 1229, 129838.	1.8	6
11463	Computational study of the effect of -spacers on the optoelectronic properties of carbazole-based organic dyes. Journal of Molecular Modeling, 2021, 27, 122.	0.8	6
11464	Rational design of a fluorescent probe for the detection of LAP and its application in drug-induced liver injury. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 251, 119362.	2.0	8
11465	Assessing the Accuracy of Local Hybrid Density Functional Approximations for Molecular Response Properties. Journal of Chemical Theory and Computation, 2021, 17, 2928-2947.	2.3	39
11466	Screening Ionic Liquids Based on Ionic Volume and Electrostatic Potential Analyses. Journal of Physical Chemistry B, 2021, 125, 3653-3664.	1.2	20
11467	In a search for potential drug candidates for combating COVID-19: computational study revealed salvianolic acid B as a potential therapeutic targeting 3CLpro and spike proteins. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8866-8893.	2.0	52
11468	Pathways for the Formation of Formamide, a Prebiotic Biomonomer: Metal-Ions in Interstellar Gas-Phase Chemistry. Journal of Physical Chemistry A, 2021, 125, 3457-3472.	1.1	8
11469	Koopmans-Type Theorem in Kohn-Sham Theory with Optimally Tuned Long-Range-Corrected (LC) Functionals. Journal of Physical Chemistry A, 2021, 125, 3489-3502.	1.1	16
11470	Understanding the role of Dimethylformamide as co-solvents in the dissolution of cellulose in ionic liquids: Experimental and theoretical approach. Journal of Molecular Liquids, 2021, 328, 115392.	2.3	19
11471	Probing the Mechanism for 2,4-Dihydroxyacetophenone Dioxygenase Using Biomimetic Iron Complexes. Inorganic Chemistry, 2021, 60, 7168-7179.	1.9	2
11472	A Spectroscopic Overview of Intramolecular Hydrogen Bonds of NH O,S,N Type. Molecules, 2021, 26, 2409.	1.7	15

#	ARTICLE	IF	CITATIONS
11473	Kinetics and mechanisms of OH-induced 2-ethoxyethanol oxidation in the atmosphere. <i>Structural Chemistry</i> , 2021, 32, 2147-2157.	1.0	3
11474	Protonation of quinoline yellow WS in aqueous solutions: Spectroscopic and DFT theoretical studies. <i>Journal of Molecular Liquids</i> , 2021, 327, 114881.	2.3	7
11475	Structure Elucidation and Confirmation of Phloroglucinols from the Roots of <i>Garcinia dauphinensis</i> by Comparison of Experimental and Calculated ECD Spectra and Specific Rotations. <i>Journal of Natural Products</i> , 2021, 84, 1163-1174.	1.5	2
11476	Anion assisted extraction of U(VI) in alkylammonium ionic liquid: Experimental and DFT studies. <i>Separation and Purification Technology</i> , 2021, 261, 118275.	3.9	8
11477	Design, synthesis, DFT, molecular modelling studies and biological evaluation of novel 3-substituted (E)-5-(arylidene)-1-methyl-2-thioxoimidazolidin-4-ones with potent cytotoxic activities against breast MCF-7, liver HepG2, and lung A549. <i>Journal of Molecular Structure</i> , 2021, 1229, 129805.	1.8	13
11478	Relationship between Hydrogen-Bonding Motifs and the $1b_{1g}$ Splitting in the X-ray Emission Spectrum of Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3996-4002.	2.1	21
11479	Strongly reducing magnesium(0) complexes. <i>Nature</i> , 2021, 592, 717-721.	13.7	86
11480	Quantum chemical calculations for the H free radical chemisorption with different chain models during oil shale pyrolysis. <i>Fuel</i> , 2021, 290, 119999.	3.4	6
11481	Synthesis and Properties of Dibenzothiophene Embedded Heteroporphyrins. <i>Journal of Organic Chemistry</i> , 2021, 86, 6100-6110.	1.7	14
11482	Multiconfiguration Density-Coherence Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2775-2782.	2.3	12
11483	Computational NMR of Carbohydrates: Theoretical Background, Applications, and Perspectives. <i>Molecules</i> , 2021, 26, 2450.	1.7	21
11484	Optical-electronic performance and mechanism investigation of dihydroindolocarbazole-based organic dyes for DSSCs. <i>Results in Physics</i> , 2021, 23, 103939.	2.0	8
11485	Binding energies and sticking coefficients of H_2 on crystalline and amorphous CO ice. <i>Astronomy and Astrophysics</i> , 2021, 648, A84.	2.1	9
11486	Unitary coupled-cluster approach for the calculation of core-excited states and x-ray absorption spectra. <i>Journal of Chemical Physics</i> , 2021, 154, 154108.	1.2	4
11487	Computational insight into the hydrogenation of CO ₂ and carbamic acids to methanol by a ruthenium(II)-based catalyst: The role of amino (NH) ligand group. <i>Molecular Catalysis</i> , 2021, 506, 111544.	1.0	4
11488	Controlling and Fine-Tuning Charge-Transfer Emission in 2,6-Dicyanoaniline Multichromophores Prepared through Domino Reactions: Entry to a Potentially New Class of OLEDs. <i>Journal of Organic Chemistry</i> , 2021, 86, 6111-6125.	1.7	7
11489	Lewis Structures from Open Quantum Systems Natural Orbitals: Real Space Adaptive Natural Density Partitioning. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4013-4025.	1.1	6
11490	Coumarin-triazole hybrids: Design, microwave-assisted synthesis, crystal and molecular structure, theoretical and computational studies and screening for their anticancer potentials against PC-3 and DU-145. <i>Journal of Molecular Structure</i> , 2021, 1230, 129899.	1.8	17

#	ARTICLE	IF	CITATIONS
11491	DFT investigation of solvent, substituent, and catalysis effects on the intramolecular Diels-Alder reaction. <i>Journal of Molecular Modeling</i> , 2021, 27, 125.	0.8	15
11492	Full optical rotation tensor at coupled cluster with single and double excitations level in the modified velocity gauge. <i>Chirality</i> , 2021, 33, 303-314.	1.3	11
11493	Embelinâ€™s Versatile Photochemistry Makes It a Potent Photosensitizer for Photodynamic Therapy. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3527-3537.	1.2	2
11494	CHAL336 Benchmark Set: How Well Do Quantum-Chemical Methods Describe Chalcogen-Bonding Interactions?. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2783-2806.	2.3	42
11495	Discovery of a novel potent cytochrome P450 CYP4Z1 inhibitor. <i>European Journal of Medicinal Chemistry</i> , 2021, 215, 113255.	2.6	13
11496	Two novel thiophene derivatives based on chalcone skeleton: a systematic study of ultrafast nonlinear absorption and excited-state dynamics. <i>Optical Materials</i> , 2021, 114, 110969.	1.7	6
11497	Multiconfiguration Pair-Density Functional Theory. <i>Annual Review of Physical Chemistry</i> , 2021, 72, 541-564.	4.8	28
11498	Benchmark calculations of proton affinity and gasâ€‘phase basicity using multilevel (<sc>G4</sc> and Tj ETQq1 1 0.784314 rgBT / Dv benzaldehyde compounds. <i>Journal of Computational Chemistry</i> , 2021, 42, 1106-1117.	1.5	8
11499	Chiral Selfâ€‘Sorting of Diformylated N â€‘Heteroâ€‘ortho â€‘phenylene Hexamers by Macrocyclization with Aromatic Diamines. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 2736-2745.	1.2	0
11500	Solubility Behavior of CO₂ in Ionic Liquids Based on Ionic Polarity Index Analyses. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3665-3676.	1.2	17
11501	Gas-Phase Experimental and Computational Studies of 5-Halouracils: Intrinsic Properties and Biological Implications. <i>Journal of Organic Chemistry</i> , 2021, 86, 6361-6370.	1.7	5
11502	Fermi-LÃ‘wdin-orbital self-interaction correction using the optimized-effective-potential method within the Krieger-Li-lafrate approximation. <i>Physical Review A</i> , 2021, 103, .	1.0	14
11503	Experimental and first-principles study of a new hydrazine derivative for DSSC applications. <i>Journal of Molecular Structure</i> , 2021, 1229, 129799.	1.8	17
11505	Computer-assisted evaluation of plant-derived Î²-secretase inhibitors in Alzheimerâ€™s disease. <i>Egyptian Journal of Medical Human Genetics</i> , 2021, 22, .	0.5	8
11506	First-Principles Nonadiabatic Dynamics Simulation of Azobenzene Photodynamics in Solutions. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3019-3030.	2.3	11
11507	Structures of Small Tantalum Cluster Anions: Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3135-3145.	1.1	9
11508	First-principles study of thermoelectric transport properties in low-buckled monolayer silicene. <i>Physica B: Condensed Matter</i> , 2021, 606, 412715.	1.3	14
11509	Exploring the Superhalogen Properties of Polynuclear Structures without Halogen Ligands: A Combined <i>Ab Initio</i> and DFT Study on Triple-Bridged [Mg₂L₅]^{âˆ’1} (L = âˆ’OCN, âˆ’SCN) Anions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3378-3386.	1.1	6

#	ARTICLE	IF	CITATIONS
11510	Synthesis of non-aromatic stable di-para-benzihomoporphyrins. <i>Tetrahedron</i> , 2021, 88, 132126.	1.0	8
11511	Exploration of superhalogen nature of Pt(CN) _n complexes (n = 1–6) and their abilities to form supersalts and superacids: a DFT–D3 study. <i>Structural Chemistry</i> , 2021, 32, 2209-2221.	1.0	5
11512	An Ion–Pairing Approach to Stereoselective Metal–Free Ring–Opening Metathesis Polymerization. <i>Angewandte Chemie</i> , 2021, 133, 14071-14077.	1.6	5
11513	Theoretical Study of Actinide(III)-DOTA Complexes. <i>ACS Omega</i> , 2021, 6, 13321-13330.	1.6	13
11514	Towards significant enhancement of structural and optoelectronic properties of porphyrin palladium(II) complex: A theoretical and experimental analysis. <i>Journal of Molecular Structure</i> , 2021, 1232, 129933.	1.8	8
11515	<i>Ab Initio</i> Excited-State Electronic Circular Dichroism Spectra Exploiting the Third-Order Algebraic-Diagrammatic Construction Scheme for the Polarization Propagator. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5132-5137.	2.1	8
11516	ParAMS: Parameter Optimization for Atomistic and Molecular Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3737-3743.	2.5	9
11517	Fluorescent Indolo[3,2- <i>a</i>]phenazines against <i>Toxoplasma gondii</i> : Concise Synthesis by Gold–Catalyzed Cycloisomerization with 1,2-Silyl Migration and <i>ipso</i> –Iodination Suzuki Sequence. <i>Chemistry - A European Journal</i> , 2021, 27, 9774-9781.	1.7	2
11518	High-Yielding Flow Synthesis of a Macrocyclic Molecular Hinge. <i>Journal of the American Chemical Society</i> , 2021, 143, 7553-7565.	6.6	13
11519	Electrocatalytic Hydrogen Evolution Catalyzed by 3,4-Toluenedithiolate Nickel Complexes of Bis(diphenylphosphine)amine Ligand Containing An Azahydrophilic Group. <i>ChemCatChem</i> , 2021, 13, 2852-2862.	1.8	2
11520	Structures of a non-ribosomal peptide synthetase condensation domain suggest the basis of substrate selectivity. <i>Nature Communications</i> , 2021, 12, 2511.	5.8	53
11521	Harmonic Infrared and Raman Spectra in Molecular Environments Using the Polarizable Embedding Model. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3599-3617.	2.3	6
11522	Vibrational Analysis of Benziodoxoles and Benziadazolotetrazaoles. <i>Physchem</i> , 2021, 1, 45-68.	0.5	5
11523	Hydroxy phenyl hydrazides and their role as corrosion impeding agent: A detail experimental and theoretical study. <i>Journal of Molecular Liquids</i> , 2021, 330, 115605.	2.3	24
11524	A guide to benchmarking enzymatically catalysed reactions: the importance of accurate reference energies and the chemical environment. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	6
11525	Isomerism in secondary bonded complexes: Do structural rules apply?. <i>International Journal of Quantum Chemistry</i> , 0, , e26670.	1.0	0
11526	Information-Theoretic Bounds on Quantum Advantage in Machine Learning. <i>Physical Review Letters</i> , 2021, 126, 190505.	2.9	98
11527	Significance Of Nuclear Quantum Effects In Hydrogen Bonded Molecular Chains. <i>ACS Nano</i> , 2021, 15, 10357-10365.	7.3	11

#	ARTICLE	IF	CITATIONS
11528	Fast and Accurate Computation of Nonadiabatic Coupling Matrix Elements Using the Truncated Leibniz Formula and Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4722-4728.	2.1	15
11529	Noncovalent Interactions from Models for the MÃllerâ€Plesset Adiabatic Connection. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4867-4875.	2.1	15
11530	Combined MD and QM/MM Investigations of Hydride Reduction of 5 α -Dihydrotestosterone Catalyzed by Human 3 α -Hydroxysteroid Dehydrogenase Type 3: Importance of Noncovalent Interactions. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4998-5008.	1.2	4
11531	Computational Studies on Reactions of Some Organic Azides with C-H Bonds. <i>ChemistrySelect</i> , 2021, 6, 4368-4381.	0.7	2
11532	Kagome phosphorene molecular device for sensing chloropicrin and phosgene â€ A first-principles study. <i>Chemical Physics Letters</i> , 2021, 771, 138472.	1.2	32
11533	<i>Bis</i> (Dibenzothiophene) Embedded Hexaphyrins: Synthesis, Structure and Properties. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 1463-1471.	1.3	4
11534	Kinetics of three reactions involving the azide radical: H \dot{A} N ₃ , thermal decomposition of N ₃ , and N ₃ \dot{A} N ₃ . <i>Chemical Physics Letters</i> , 2021, 771, 138515.	1.2	0
11535	Pressure induced semiconductor to metal phase transition in cubic CsSnBr ₃ perovskite. <i>AIP Advances</i> , 2021, 11, .	0.6	29
11536	New 3-Ethynylaryl Coumarin-Based Dyes for DSSC Applications: Synthesis, Spectroscopic Properties, and Theoretical Calculations. <i>Molecules</i> , 2021, 26, 2934.	1.7	12
11537	Computational Study of Key Mechanistic Details for a Proposed Copper (I)-Mediated Deconstructive Fluorination of N-Protected Cyclic Amines. <i>Topics in Catalysis</i> , 2022, 65, 418-432.	1.3	4
11538	Kinetic resolution of racemic 6-substituted 1,2,3,4-tetrahydroquinolines with chiral acyl chlorides. Experiment and quantum chemical simulation. <i>Russian Chemical Bulletin</i> , 2021, 70, 890-899.	0.4	4
11539	Magnesium and Nickel Complexes with Bis(p-iminoquinone) Redox-Active Ligand. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2021, 47, 307-318.	0.3	2
11540	Analysis of Relationship Between Some Disazo Dyes Derived from 2,4-Dihydroxyquinoline and Its Anticancer and DNA Binding Properties by Density Functional Theory. <i>SDU Journal of Science</i> , 0, , 200-215.	0.1	0
11541	Theoretical prediction of an NXeH ₄ ⁺ ion with N-Xe triple bond. <i>Computational and Theoretical Chemistry</i> , 2021, 1199, 113193.	1.1	2
11542	Formation of Co(II), Ni(II), Zn(II) complexes of alternative metal binding heptapeptides and nitrilotriacetic acid: Discovering new potential affinity tags. <i>International Journal of Mass Spectrometry</i> , 2021, 463, 116554.	0.7	7
11543	Assessing the Accuracy of the SCAN Functional for Water through a Many-Body Analysis of the Adiabatic Connection Formula. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3739-3749.	2.3	13
11544	Quenching-Resistant Solid-State Photoluminescence of Graphene Quantum Dots: Reduction of $\dot{I}e\dot{a}$ Stacking by Surface Functionalization with POSS, PEG, and HDA. <i>Advanced Functional Materials</i> , 2021, 31, 2102741.	7.8	45
11545	Correlating Ultrafast Dynamics, Liquid Crystalline Phases, and Ambipolar Transport in Fluorinated Benzothiadiazole Dyes. <i>Advanced Electronic Materials</i> , 2021, 7, 2100186.	2.6	2

#	ARTICLE	IF	CITATIONS
11546	A Key Piece in the Global N-Cycle: The N ¹⁵ Bond Formation Presented by Heme-Dependent Hydrazine Synthase. <i>ACS Catalysis</i> , 2021, 11, 6489-6498.	5.5	9
11547	Accurate Electronic Excitation Energies in Full-Valence Active Space via Bootstrap Embedding. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3335-3347.	2.3	8
11548	Characterization of Thorium-Pyrazinoic acid complexation and its decorporation efficacy in human cells and blood. <i>Chemosphere</i> , 2021, 271, 129547.	4.2	5
11549	An Ion-Pairing Approach to Stereoselective Metal-Free Ring-Opening Metathesis Polymerization. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 13952-13958.	7.2	14
11550	In situ ligand formation-driven synthesis of two acylhydrazide compounds: Synthesis, structure and photoluminescence properties. <i>Inorganica Chimica Acta</i> , 2021, 519, 120269.	1.2	0
11551	Structures and thermal decomposition of complexes of E(C ₆ F ₅) ₃ (E = Al, Ga, In) with pyridine. <i>Journal of Organometallic Chemistry</i> , 2021, 948, 121909.	0.8	5
11553	Multiferroic ground states in free standing perovskite-based nanodots: a density functional theory study. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2021, 29, 055002.	0.8	1
11554	Effects of Multiple OH/SH Substitution on the Bonding/Stability versus Aromaticity of Benzene Rings: From Computational Insights. <i>ChemistrySelect</i> , 2021, 6, 5120-5139.	0.7	6
11555	Strained Ruthenium Complexes Bearing Tridentate Guanidine-Derived Ligands. <i>Helvetica Chimica Acta</i> , 2021, 104, e2100044.	1.0	3
11556	Exploring the Size-Dependent Hydrogen Storage Property on Ti-Doped B ₂ Clusters by Diatomic Deposition: Temperature Controlled H ₂ Release. <i>Advanced Theory and Simulations</i> , 2021, 4, 2100043.	1.3	8
11557	Functionalized Au ₁₅ nanoclusters as luminescent probes for protein carbonylation detection. <i>Communications Chemistry</i> , 2021, 4, .	2.0	16
11558	Photoinduced Release of Volatile Organic Compounds from Fatty Alcohols at the Air-Water Interface: The Role of Singlet Oxygen Photosensitized by a Carbonyl Group. <i>Environmental Science & Technology</i> , 2021, 55, 8683-8690.	4.6	28
11560	Design of New Schiff-Base Copper(II) Complexes: Synthesis, Crystal Structures, DFT Study, and Binding Potency toward Cytochrome P450 3A4. <i>ACS Omega</i> , 2021, 6, 13704-13718.	1.6	64
11561	Carbazole derivatives: Synthesis, spectroscopic characterization, antioxidant activity, molecular docking study, and the quantum chemical calculations. <i>Journal of Molecular Liquids</i> , 2021, 330, 115651.	2.3	24
11562	Isolation and structural elucidation of novel fusococcan dehydroxypericonin A from <i>Roussoella</i> sp. <i>Bioscience, Biotechnology and Biochemistry</i> , 2021, 85, 1798-1801.	0.6	1
11563	Investigation of lanthanide complexation with acetohydroxamic acid in nitrate medium: experimental and DFT studies. <i>Journal of Chemical Sciences</i> , 2021, 133, 1.	0.7	2
11564	On the relation between oxidation states and d-electron populations of the 1st row transition metal complexes I. Tetrachloro complexes. <i>Polyhedron</i> , 2021, 201, 115172.	1.0	4
11565	Exploration of N-oxo pyridine 2-carboxamide ligands towards coordination chemistry, solvent extraction, and DFT investigation for the development of novel solvent for lanthanide and actinide separation. <i>Polyhedron</i> , 2021, 201, 115166.	1.0	5

#	ARTICLE	IF	CITATIONS
11566	Benchmark of the Extension of Frozen-Density Embedding Theory to Nonvariational Correlated Methods: The Embedded-MP2 Case. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4049-4062.	2.3	4
11567	Chlorobenzene and 1, 4-dichlorobenzene adsorption studies on $\hat{\text{I}}$ -Arsenene nanosheet – a first-principles analysis. <i>Molecular Physics</i> , 2021, 119, e1936248.	0.8	11
11568	Synergistic interaction of N-3-(3-Bromobenzyl)-N-oxycapine and docetaxel abrogates oncogenic potential of breast cancer cells. <i>Chemical Biology and Drug Design</i> , 2021, 98, 466-479.	1.5	6
11569	Multimolecular complexes of the phosphodiester anion with Zn(II) or Mg(II) and water molecules – Preliminary validations of a polarizable potential by ab initio quantum chemistry. <i>Journal of Computational Chemistry</i> , 2021, 42, 1430-1446.	1.5	0
11570	Attractive and repulsive residue fragments at the interface of SARS-CoV-2 and hACE2. <i>Scientific Reports</i> , 2021, 11, 12567.	1.6	5
11571	An ab initio study on the dynamical properties of U-Nb alloy melt. <i>Chinese Physics B</i> , 0, , .	0.7	0
11572	Sensitivity of the Fermi surface to the treatment of exchange and correlation. <i>Physical Review B</i> , 2021, 103, .	1.1	3
11574	Generation, Characterization, and Dissociation of Radical Cations Derived from Prolyl-glycyl-glycine. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6121-6129.	1.2	1
11575	A theoretical investigation of complexation for pyrimidine bases with Hg ²⁺ and Cd ²⁺ by DFT method. <i>Nanotechnology for Environmental Engineering</i> , 2021, 6, 1.	2.0	1
11576	Tuning the electronic and optical properties of Blue P/MoSeS and Blue P/MoSSe van der Waals heterostructure via biaxial strain. <i>Chemical Physics Letters</i> , 2021, 773, 138622.	1.2	4
11577	Reaction pathways and cyclic chain model of free radicals during coal spontaneous combustion. <i>Fuel</i> , 2021, 293, 120436.	3.4	65
11578	Systematic improvement of molecular excited state calculations by inclusion of nuclear quantum motion: A mode-resolved picture and the effect of molecular size. <i>Journal of Chemical Physics</i> , 2021, 154, 244109.	1.2	5
11579	Molecular structure, vibrational spectroscopic, frontier molecular orbital and natural bond orbital analysis of anti-cancer drug 6-chloro-3- pyridine carbonitrile. <i>Spectroscopy Letters</i> , 2021, 54, 419-436.	0.5	8
11580	Enzymatic N N bond formation: Mechanism for the N-nitroso synthesis catalyzed by non-heme iron SznF enzyme. <i>Journal of Catalysis</i> , 2021, 398, 44-53.	3.1	7
11581	Band gaps of liquid water and hexagonal ice through advanced electronic-structure calculations. <i>Physical Review Research</i> , 2021, 3, .	1.3	20
11582	Theoretical investigation of benzo(a)pyrene formation. <i>Chemical Physics Letters</i> , 2021, 772, 138564.	1.2	14
11583	Multireference calculations on the ground and lowest excited states and dissociation energy of LuF. <i>Journal of Chemical Physics</i> , 2021, 154, 244304.	1.2	4
11584	A Formal Rearrangement of Allylic Silanols. <i>Molecules</i> , 2021, 26, 3829.	1.7	10

#	ARTICLE	IF	CITATIONS
11585	Tethered Silanoxyiodination of Alkenes. <i>Journal of Organic Chemistry</i> , 2021, 86, 9233-9243.	1.7	10
11586	A tautomeric ligand enables directed C-H hydroxylation with molecular oxygen. <i>Science</i> , 2021, 372, 1452-1457.	6.0	84
11587	Optical features of ligated semiconducting quantum dots subjected to an electric field. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26763.	1.0	1
11588	Evaluation of density functional theory for a large and diverse set of organic and inorganic equilibrium structures. <i>Journal of Computational Chemistry</i> , 2021, 42, 1590-1601.	1.5	44
11589	The corrosion inhibition and adsorption behavior of mercaptobenzimidazole and bis-mercaptobenzimidazole on carbon steel in 1.0 M HCl: Experimental and computational insights. <i>Surfaces and Interfaces</i> , 2021, 24, 101095.	1.5	36
11590	Structural and electronic properties of organophosphorus-based systems as sensitizers in solar cells. <i>Materials Today Chemistry</i> , 2021, 20, 100469.	1.7	2
11591	Borataalkene Hydrofunctionalization Reactions. <i>Organometallics</i> , 2021, 40, 1966-1973.	1.1	6
11592	Performance of the DLPNO-CCSD and recent DFT methods in the calculation of isotropic and dipolar contributions to ¹⁴ N hyperfine coupling constants of nitroxide radicals. <i>Journal of Molecular Modeling</i> , 2021, 27, 194.	0.8	3
11593	Using Atomic Charges to Describe the ρ of Carboxylic Acids. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2733-2743.	2.5	18
11594	Assessing locally range-separated hybrid functionals from a gradient expansion of the exchange energy density. <i>Journal of Chemical Physics</i> , 2021, 154, 214101.	1.2	10
11595	Perturbation approach to constrained electron transfer in density functional theory. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	1
11596	Determination of electronic characteristics of tetrahydro pyrimidine derivatives and investigation of usability as anti-corrosion. <i>International Journal of Chemistry and Technology</i> , 0, , .	0.8	0
11597	Theoretical Study of Effects of Solvents, Ligands, and Anions on Separation of Trivalent Lanthanides and Actinides. <i>Inorganic Chemistry</i> , 2021, 60, 9552-9562.	1.9	14
11598	Relating molecular descriptors to frontier orbital energy levels, singlet and triplet excited states of fused tricyclics using machine learning. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107891.	1.3	5
11599	A novel BODIPY-based fluorescent probe for sensitive and selective detection of nerve agent simulants through base-assisted photo-induced electron transfer process. <i>Sensors and Actuators B: Chemical</i> , 2021, 337, 129804.	4.0	17
11600	Experimental and theoretical analysis of molecular structure, vibrational spectra and biological properties of the new Co(II), Ni(II) and Cu(II) Schiff base metal complexes. <i>Journal of Molecular Structure</i> , 2021, 1233, 130097.	1.8	37
11601	Iron-Catalyzed Halogen Exchange of Trifluoromethyl Arenes**. <i>Chemistry - A European Journal</i> , 2021, 27, 10839-10843.	1.7	7
11602	Super selective ammonia separation through multiple-site interaction with ionic liquid-based hybrid membranes. <i>Journal of Membrane Science</i> , 2021, 628, 119264.	4.1	31

#	ARTICLE	IF	CITATIONS
11603	Experimental methods in chemical engineering: Density functional theory. Canadian Journal of Chemical Engineering, 2021, 99, 1885-1911.	0.9	19
11604	Perimeter Coordinated Diastereomeric Rh(I) Complex of Helically Twisted Weakly Aromatic Hybrid Singly N-Confused P^2P^2 Fused Ferrocenoporphyrinoids. Journal of Organic Chemistry, 2021, 86, 8015-8026.	1.7	8
11605	Theoretical isotope fractionation of cadmium during complexation with organic ligands. Chemical Geology, 2021, 571, 120178.	1.4	28
11606	Synthesis of one-component type II dithioxanthone-disulfide photoinitiator and investigation of photophysical and photochemical properties. European Polymer Journal, 2021, 153, 110510.	2.6	5
11607	Boyaya Duyarl \pm G $\frac{1}{4}$ ne \ddot{Y} Pillerinde Trifenilamin Tabanl \pm Organik Boyalar \pm n Kuantum Kimyasal Hesaplamalar \pm . Caucasian Journal of Science, 0, , .	0.2	0
11608	A DFT Study on Structures and Electronic Properties of Iron(II) Terpyridyltriphenylamine Derivatives. Russian Journal of Physical Chemistry A, 2021, 95, 1177-1184.	0.1	0
11609	Sensing capability and diameter-dependent electronic structure of boron nitride nanotubes. Materials Today Communications, 2021, 27, 102252.	0.9	8
11610	Enantioselective Catalytic Dearomative Addition of Grignard Reagents to 4-Methoxypyridinium Ions. ACS Catalysis, 2021, 11, 8476-8483.	5.5	26
11611	Structural, Electronic, and Nonlinear Optical Properties of C ₆ H ₄ and C ₇ OCl ₆ Encapsulating Li and F Atoms. ACS Omega, 2021, 6, 16234-16240.	1.6	4
11612	Comparison of (5 + 2) Cycloadditions Involving Oxidopyrylium and Oxidopyridinium Ions: Relative Reactivities. Journal of Organic Chemistry, 2021, 86, 8652-8659.	1.7	6
11613	Mechanism-Based Insights into Removing the Mutagenicity of Aromatic Amines by Small Structural Alterations. Journal of Medicinal Chemistry, 2021, 64, 8545-8563.	2.9	7
11614	Rational design of $\langle \text{pincer} \text{ nickel} \rangle$ complexes for catalytic cyanomethylation of benzaldehyde: A systematic $\langle \text{DFT} \rangle$ study. Journal of Computational Chemistry, 2021, 42, 1728-1735.	1.5	5
11615	Anticorrosive and antioxidant effect of the aqueous extract of the leaves, flowers, and stems of Cistus monspeliensis L: Experimental and computational study. Journal of Molecular Liquids, 2021, 331, 115771.	2.3	12
11616	Intercalation Ability of Novel Monofunctional Platinum Anticancer Drugs: A Key Step in Their Biological Action. Journal of Chemical Information and Modeling, 2021, 61, 4391-4399.	2.5	9
11617	Molecular structure aspects and molecular reactivity of some triazole derivatives for corrosion inhibition of aluminum in 1M HCl solution. Journal of Molecular Structure, 2021, 1236, 130292.	1.8	45
11618	Benzocarbazole-based $\text{D}^{\text{A}}\text{D}^{\text{A}}\text{A}$ dyes for DSSCs: DFT/TD-DFT study of influence of auxiliary donors on the performance of free dye and dye TiO_2 interface. Research on Chemical Intermediates, 2021, 47, 4257-4280.	1.3	31
11619	Combustion chemistry of methoxymethanol. Part I: Chemical kinetics of hydrogen-abstraction reactions and the unimolecular reactions of the product [C ₂ H ₅ O ₂] radicals. Combustion and Flame, 2021, 229, 111396.	2.8	10
11620	Decaspirones and palmarumycins from Phaeoseptum sp. KT4106: Chirality reinvestigation of palmarumycins CP4a and CP5. Tetrahedron, 2021, 92, 132251.	1.0	3

#	ARTICLE	IF	CITATIONS
11621	Combined crossed molecular beams and computational study on the $N(\text{D})^+ + \text{HCCCN}(X) \rightarrow \text{N}^+ + \text{C}_2\text{H}_2$ reaction and implications for extra-terrestrial environments. <i>Molecular Physics</i> , 2022, 120, .	0.8	9
11622	Complexation of <i>C</i> -Functionalized Cyclams with Copper(II) and Zinc(II): Similarities and Changes When Compared to Parent Cyclam Analogues. <i>Inorganic Chemistry</i> , 2021, 60, 10857-10872.	1.9	10
11623	Exact-two-component block-localized wave function: A simple scheme for the automatic computation of relativistic \hat{H}^{SCF} . <i>Journal of Chemical Physics</i> , 2021, 155, 014103.	1.2	5
11624	Investigation of kinetics of phenyl radicals with ethyl formate in the gas phase using cavity ring-down spectroscopy and theoretical methodologies. <i>Photochemical and Photobiological Sciences</i> , 2021, 20, 859-873.	1.6	1
11625	Performing Molecular Dynamics Simulations and Computing Hydration Free Energies on the B3LYP-D3(BJ) Potential Energy Surface with Adaptive Force Matching: A Benchmark Study with Seven Alcohols and One Amine. <i>ACS Physical Chemistry Au</i> , 2021, 1, 14-24.	1.9	9
11626	First-Principles Calculations of the Protonation and Weakening of Epoxy Resin under Wet Conditions. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8989-8996.	1.2	8
11627	Amphipathic Barbiturates as Mimics of Antimicrobial Peptides and the Marine Natural Products Eusynstyelamides with Activity against Multi-resistant Clinical Isolates. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 11395-11417.	2.9	22
11628	Evaluation of optical band gaps and dopant state energies in transition metal oxides using oxidation-state constrained density functional theory. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 365901.	0.7	3
11629	Unraveling the Interaction of Water-in-Oil Emulsion Droplets via Molecular Simulations and Surface Force Measurements. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7556-7567.	1.2	8
11630	Osmium Arene Germyl, Stannyl, Germanate, and Stannate Complexes as Anticancer Agents. <i>ACS Omega</i> , 2021, 6, 19252-19268.	1.6	5
11631	Computational investigation of interaction between titanocene dichloride and nanoclusters (B12N12). <i>Tj ETQq0 0 0 rgBT /Overlock 10 T</i>	0.4	3
11632	Evidence of Critical Tunnelling Width in Ensuring Spin Polarized Asymmetric Negative Differential Resistance Feature in Two-Dimensional $g^{\text{C}}_4 \text{N}_3$ graphene- $g^{\text{C}}_4 \text{N}_3$. <i>ChemistrySelect</i> , 2021, 6, 6916-6924.	0.7	0
11633	Electronic Properties of Ti Sites in Ziegler-Natta Catalysts. <i>ACS Catalysis</i> , 2021, 11, 9949-9961.	5.5	32
11634	Surface-Promoted Evolution of Ru-bda Coordination Oligomers Boosts the Efficiency of Water Oxidation Molecular Anodes. <i>Journal of the American Chemical Society</i> , 2021, 143, 11651-11661.	6.6	28
11635	H_2 Evolution from Electrocatalysts with Redox-Active Ligands: Mechanistic Insights from Theory and Experiment vis-À-vis Co-Mabiq. <i>Inorganic Chemistry</i> , 2021, 60, 13888-13902.	1.9	7
11636	Adsorption of methylene blue cationic dye onto brookite and rutile phases of titanium dioxide: Quantum chemical and molecular dynamic simulation studies. <i>Inorganic Chemistry Communication</i> , 2021, 129, 108659.	1.8	21
11637	Mechanism and kinetic study for the reaction of allyl cyanide with Cl atom in the presence of O ₂ . <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113286.	1.1	1
11638	An improved Slater's transition state approximation. <i>Journal of Chemical Physics</i> , 2021, 155, 034101.	1.2	12

#	ARTICLE	IF	CITATIONS
11639	The Ionization Energies of Dust-Forming Metal Oxide Clusters. <i>Universe</i> , 2021, 7, 243.	0.9	4
11640	Perturbation Theory Treatment of Spin-Orbit Coupling II: A Coupled Perturbed Kohn-Sham Method. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4712-4732.	2.3	7
11641	A Schiff base-functionalized graphene quantum dot nanocomposite for preferable picric acid sensing. <i>Dyes and Pigments</i> , 2021, 191, 109355.	2.0	30
11642	BODIPY-Pyridylhydrazone Probe for Fluorescence Turn-On Detection of Fe ³⁺ and Its Bioimaging Application. <i>Chemosensors</i> , 2021, 9, 165.	1.8	13
11643	Theoretical study of the Diels-Alder reaction of 3-bromo-1-phenylprop-2-ynone with furan and 2-methylfuran. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	5
11644	Heme ligation in the gas phase. <i>International Reviews in Physical Chemistry</i> , 2021, 40, 365-404.	0.9	2
11645	Synthesis, identification, density functional and Hirshfeld surface studies of 2,2'-disulfanediybis() Tj ETQq0 0 0 rgBT /Overlock 10 T 2021, 42, 1873-1884.	1.5	1
11647	Realization of Flexible Ultraviolet Organic Light-Emitting Diodes: Key Design Issues. <i>Advanced Photonics Research</i> , 2021, 2, 2100108.	1.7	4
11648	Plausible Pnictogen Bonding of epi-Cinchonidine as a Chiral Scaffold in Catalysis. <i>Frontiers in Chemistry</i> , 2021, 9, 669515.	1.8	7
11649	Design of High-Performance Pyridine/Quinoline Hydrazone Photoswitches. <i>Journal of Organic Chemistry</i> , 2021, 86, 11633-11646.	1.7	6
11650	Insights into the functional divergence of the haloacid dehalogenase superfamily from phosphomonoesterase to inorganic pyrophosphatase. <i>Archives of Biochemistry and Biophysics</i> , 2021, 705, 108896.	1.4	2
11651	Guided Ion Beam Studies of the Thorium Monocarbonyl Cation Bond Dissociation Energy and Theoretical Unveiling of Different Isomers of [Th ₂ O ₂ C] ⁺ and Their Rearrangement Mechanism. <i>Inorganic Chemistry</i> , 2021, 60, 10426-10438.	1.9	5
11652	Arc Synthesis, Crystal Structure, and Photoelectrochemistry of Copper(I) Tungstate. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 32865-32875.	4.0	11
11653	Efficient workflow for the investigation of the catalytic cycle of water oxidation catalysts: Combining $\langle \text{scp} \rangle$ GFN \times TB $\langle \text{scp} \rangle$ and density functional theory. <i>Journal of Computational Chemistry</i> , 2021, 42, 1885-1894.	1.5	11
11654	DFT/TD-DFT Study of Donor-Acceptor Organic Dye models contained Triarylamine for an Efficient Dye-Sensitized Solar Cell. <i>Journal of Physics: Conference Series</i> , 2021, 1963, 012012.	0.3	3
11655	Selfconsistent random phase approximation methods. <i>Journal of Chemical Physics</i> , 2021, 155, 040902.	1.2	16
11656	Impact of the Characteristics of Quantum Chemical Databases on Machine Learning Prediction of Tautomerization Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4769-4785.	2.3	12
11657	CO ₂ Activation Within a Superalkali-Doped Fullerene. <i>Frontiers in Chemistry</i> , 2021, 9, 712960.	1.8	3

#	ARTICLE	IF	CITATIONS
11658	First-principles correction scheme for linear-response time-dependent density functional theory calculations of core electronic states. <i>Journal of Chemical Physics</i> , 2021, 155, 034108.	1.2	7
11659	Analyzing Hydration Differences in Cocrystal Polymorphs: High-Resolution X-ray Investigation of Caffeine-Glutaric Acid Cocrystals. <i>Crystal Growth and Design</i> , 2021, 21, 4456-4467.	1.4	5
11660	Density Functional Geometries and Zero-Point Energies in Ab Initio Thermochemical Treatments of Compounds with First-Row Atoms (H, C, N, O, F). <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4872-4890.	2.3	22
11661	Benchmarking of Density Functionals for <i>Z</i> -Azoarene Half-Lives via Automated Transition State Search. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6474-6485.	1.1	8
11662	Comparison in optoelectronic properties of triphenylamine-imidazole or imidazole as donor for dye-sensitized solar cell: theoretical approach. <i>Journal of Molecular Modeling</i> , 2021, 27, 225.	0.8	3
11663	Structural, Magnetic, and Dielectric Properties of Sn-Doped BiFeO ₃ : Experiment and DFT Analysis. <i>Journal of Superconductivity and Novel Magnetism</i> , 2021, 34, 2179-2188.	0.8	2
11664	Impact of Changing the Core in Tetrapyrrolic Dendrimers Designed for Oxygen Sensitization: New Fluorescent Phthalocyanine-Based Dendrimers with High Two-Photon Absorption Cross-sections. <i>Macromolecules</i> , 2021, 54, 6726-6744.	2.2	7
11665	Mechanistic Insights into Iron-Catalyzed C-H Bond Activation and C-C Coupling. <i>Organometallics</i> , 2021, 40, 2467-2477.	1.1	8
11666	Solving the strong-correlation problem in materials. <i>Rivista Del Nuovo Cimento</i> , 2021, 44, 597-640.	2.0	11
11667	The Beginning of HCN Polymerization: Iminoacetonitrile Formation and Its Implications in Astrochemical Environments. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 2152-2159.	1.2	13
11668	Assessment of Computational Methods for Calculating Accurate Non-covalent Interaction Energies in 1,2,3,5-Dithiadiazolyl Radicals. <i>Crystal Growth and Design</i> , 2021, 21, 4878-4891.	1.4	5
11669	Photochemical Deracemization of Primary Allene Amides by Triplet Energy Transfer: A Combined Synthetic and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2021, 143, 11209-11217.	6.6	55
11670	Cross-Sphere Electrode Reaction: The Case of Hydroxyl Desorption during the Oxygen Reduction Reaction on Pt(111) in Alkaline Media. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6448-6456.	2.1	7
11671	Doping alkali metal ions and introducing electron donor groups to fulleropyrrolidine derivatives: Large second-order nonlinear optical responses. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113254.	1.1	1
11672	A New Insight into Non-covalent Interactions in 1,4-Disubstituted 1H-1,2,3-Triazole: Synthesis, X-ray structure, DFT calculations, in vitro Lipoxigenase Inhibition (LOX) and in silico Studies. <i>Journal of Molecular Structure</i> , 2021, 1236, 130283.	1.8	12
11673	Assessment and prediction of band edge locations of nitrides using a self-consistent hybrid functional. <i>Journal of Chemical Physics</i> , 2021, 155, 024120.	1.2	1
11674	Description of Sudden Polarization in the Excited Electronic States with an Ensemble Density Functional Theory Method. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5123-5139.	2.3	7
11675	The ligand-to-metal charge transfer excited state of [Re(dmpe) ₃] ²⁺ . <i>Photosynthesis Research</i> , 2022, 151, 155-161.	1.6	4

#	ARTICLE	IF	CITATIONS
11676	Examination of How Well Long-Range-Corrected Density Functionals Satisfy the Ionization Energy Theorem. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4823-4830.	2.3	17
11677	Reaction Path-Force Matching in Collective Variables: Determining Ab Initio QM/MM Free Energy Profiles by Fitting Mean Force. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4961-4980.	2.3	14
11678	Computational Modeling: Theoretical Predictive Tools for Designing of Potential Organic Corrosion Inhibitors. <i>Journal of Molecular Structure</i> , 2021, 1236, 130294.	1.8	54
11679	Electrocoagulation/oxidation/flotation by direct pulsed current applied to the removal of antibiotics from Brazilian WWTP effluents. <i>Electrochimica Acta</i> , 2021, 388, 138499.	2.6	25
11680	BODIPY-Based Photodynamic Agents for Exclusively Generating Superoxide Radical over Singlet Oxygen. <i>Angewandte Chemie</i> , 2021, 133, 20065-20073.	1.6	14
11681	Rotational and Vibrational Signatures of Astrophysically relevant Gas-Phase Stereo-isomeric Species of Proteinogenic Amino acid Leucine. <i>Life Sciences in Space Research</i> , 2021, 30, 29-38.	1.2	0
11682	Boson Subsidiary Solver (BoSS) v1.1. <i>Computer Physics Communications</i> , 2021, 265, 107991.	3.0	5
11683	Ab-Initio Molecular Dynamics Simulation of the Electrolysis of Nucleobases. <i>Energies</i> , 2021, 14, 5021.	1.6	1
11684	Theoretical computations on the efficiency of acetaldehyde formation on interstellar icy grains. <i>Astronomy and Astrophysics</i> , 2021, 655, A9.	2.1	18
11685	A Statistically Supported Antioxidant Activity DFT Benchmark—The Effects of Hartree–Fock Exchange and Basis Set Selection on Accuracy and Resources Uptake. <i>Molecules</i> , 2021, 26, 5058.	1.7	21
11686	Density Functional Theory for Electrocatalysis. <i>Energy and Environmental Materials</i> , 2022, 5, 157-185.	7.3	95
11687	Product Detection of the CH ₂ Radical Reaction with Cyclopentadiene: A Novel Route to Benzene. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6927-6939.	1.1	6
11688	Photo-Induced Partially Aromatized Intramolecular Charge Transfer. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9268-9285.	1.2	12
11689	Development of Mg/Al/Si/O ReaxFF Parameters for Magnesium Aluminosilicate Glass Using an Artificial Neural Network-Assisted Genetic Algorithm. <i>Journal of Physical Chemistry C</i> , 2021, 125, 18380-18394.	1.5	13
11690	Thermoelectric performance of silicene under uniform biaxial strain: A first principles study. <i>Superlattices and Microstructures</i> , 2021, 156, 106944.	1.4	6
11691	Cross-Dimerization of 2,5-Dihydrofuran with Conjugated Dienes Catalyzed by (Chiral) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 147 3370-3388.	1.1	3
11692	The PtSe ₂ /GaN van der Waals heterostructure photocatalyst with type II alignment: A first-principles study. <i>Applied Catalysis A: General</i> , 2021, 624, 118332.	2.2	34
11693	Density Functional Theory Study on the ¹⁹³ Ir Mössbauer Spectroscopic Parameters of Vaska's Complexes and Their Oxidative Adducts. <i>Inorganic Chemistry</i> , 2021, 60, 12740-12752.	1.9	3

#	ARTICLE	IF	CITATIONS
11694	Thermal and Mechanochemical Tuning of the Porphyrin Singlet-Triplet Gap for Selective Energy Transfer Processes: A Molecular Dynamics Approach. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5429-5439.	2.3	7
11695	Radical 1,4-Aryl Migration Enabled Remote Cross-Electrophile Coupling of α -Amino β -Bromo Acid Esters with Aryl Bromides. <i>Angewandte Chemie</i> , 2021, 133, 21530-21537.	1.6	1
11696	Electronic structure and first hyperpolarizability of triple helicene compounds. <i>Journal of Molecular Structure</i> , 2021, 1237, 130332.	1.8	4
11697	Synthesis, Crystal Structure, Hirshfeld Surface Analysis, and Computational Study of a Novel Organic Salt Obtained from Benzylamine and an Acidic Component. <i>ACS Omega</i> , 2021, 6, 22357-22366.	1.6	66
11698	Double excitations in molecules from ensemble density functionals: Theory and approximations. <i>Physical Review A</i> , 2021, 104, .	1.0	10
11699	Tunable electronic and optical properties of new two-dimensional Blue P/MoSe ₂ van der Waals heterostructures with the potential for photocatalysis applications. <i>Chemical Physics Letters</i> , 2021, 777, 138740.	1.2	4
11700	SAR11 Cells Rely on Enzyme Multifunctionality To Metabolize a Range of Polyamine Compounds. <i>MBio</i> , 2021, 12, e0109121.	1.8	10
11701	Quinone Reduction by Organo-Osmium Half-Sandwich Transfer Hydrogenation Catalysts. <i>Organometallics</i> , 2021, 40, 3012-3023.	1.1	8
11702	Quantum Mechanistic Studies of the Oxidation of Ethylene by Rhenium Oxo Complexes. <i>Journal of Chemistry</i> , 2021, 2021, 1-11.	0.9	3
11703	Density functionals with full nonlocal exchange, nonlocal $r_{\text{ng}}^{\text{3.5}}$ correlation, and $\langle \text{D3} \rangle$ dispersion: Combined accuracy for general main-group thermochemistry, kinetics, and noncovalent interactions. <i>Journal of Computational Chemistry</i> , 2021, 42, 1974-1981.	1.5	2
11704	Assessment of the Accuracy of DFT-Predicted Li ⁺ Nucleic Acid Binding Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5392-5408.	2.3	4
11705	Quantum-electrodynamical time-dependent density functional theory within Gaussian atomic basis. <i>Journal of Chemical Physics</i> , 2021, 155, 064107.	1.2	29
11706	Effect of alkali atom doping on the electronic structure and aromatic character of planar and quasi-planar Al ₁₃ ⁺ clusters. <i>Journal of Molecular Modeling</i> , 2021, 27, 235.	0.8	2
11707	Red tricycle phosphorene nanoribbon as a removing medium of sulfadiazine and sulfamethoxazole molecules based on first-principles studies. <i>Journal of Molecular Liquids</i> , 2021, 336, 116294.	2.3	30
11708	A Bioinspired Ni ^{II} Superoxide Dismutase Catalyst Designed on an ATCUN-like Binding Motif. <i>Inorganic Chemistry</i> , 2021, 60, 12772-12780.	1.9	7
11709	A first-principles evaluation on the interaction of 1,3,4-oxadiazole with pristine and B-, Al-, Ga-doped C ₆₀ fullerenes. <i>Journal of Molecular Liquids</i> , 2021, 335, 116181.	2.3	34
11710	Comparison of the accuracy of DFT methods for reactions with relevance to nitrogenase. <i>Electronic Structure</i> , 2021, 3, 034005.	1.0	9
11711	Considering Density Functional Approaches for Actinide Species: The An ₆₆ Molecule Set. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7029-7037.	1.1	20

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11712	Synthesis, Molecular Structure, HOMO-LUMO, Chemical, Spectroscopic (UV-Vis and IR), Thermochemical Study of Ethyl 6-amino-5-cyano-2-methyl-4-(4-nitrophenyl)-4H-pyran-3-carboxylate: A DFT Exploration. <i>Material Science Research India</i> , 2021, 18, 179-189.	0.9	1
11713	Band gaps of crystalline solids from Wannier-localizationâ€‘based optimal tuning of a screened range-separated hybrid functional. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	49
11714	Oxidative decomposition and mineralization of caffeine by advanced oxidation processes: The effect of hybridization. <i>Ultrasonics Sonochemistry</i> , 2021, 76, 105635.	3.8	10
11715	The microscopic insights into the adsorption of Cu ²⁺ , Pb ²⁺ and Zn ²⁺ onto g-C ₃ N ₄ surfaces by a combined spectroscopic characterization and DFT theoretical calculations. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 105433.	3.3	6
11716	Structureâ€‘based virtual screening and computational study towards identification of novel inhibitors of hypoxanthineâ€‘guanine phosphoribosyltransferase of <i>Trypanosoma cruzi</i> . <i>Journal of Cellular Biochemistry</i> , 2021, 122, 1701-1714.	1.2	2
11717	BODIPYâ€‘Based Photodynamic Agents for Exclusively Generating Superoxide Radical over Singlet Oxygen. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 19912-19920.	7.2	186
11718	Tuning the structural and catalytic properties of copper(II)-based complexes containing pyridine-2,6-diimines. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 10677-10695.	2.0	2
11719	Ru(0)-Catalyzed Synthesis of Borylated-Conjugated Triene Building Blocks by Cross-Dimerization and Their Use in Cross-Coupling Reactions. <i>Bulletin of the Chemical Society of Japan</i> , 2021, 94, 2113-2132.	2.0	8
11720	Extrapolating DFT Toward the Complete Basis Set Limit: Lessons from the PBE Family of Functionals. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5651-5660.	2.3	14
11721	Identification of the Key Parameters for Horizontal Transition Dipole Orientation in Fluorescent and TADF Organic Lightâ€‘Emitting Diodes. <i>Advanced Materials</i> , 2021, 33, e2100677.	11.1	99
11722	Efficient Approximation of Potential Energy Surfaces with Mixed-Basis Interpolation. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5673-5683.	2.3	3
11723	Investigation of electrochemical oxidative coupling of 3 and 6 substituted carbazoles. <i>Journal of Electroanalytical Chemistry</i> , 2021, 894, 115356.	1.9	5
11724	A New Solid-State Proton Conductor: The Salt Hydrate Based on Imidazolium and 12-Tungstophosphate. <i>Journal of the American Chemical Society</i> , 2021, 143, 13895-13907.	6.6	28
11725	On assessing functional errors in density functional theory using atomisation energies and electric field gradients. <i>International Journal of Quantum Chemistry</i> , 0, , e26799.	1.0	1
11726	Computational Screening of Chiral Organic Semiconductors: Exploring Side-Group Functionalization and Assembly to Optimize Charge Transport. <i>Crystal Growth and Design</i> , 2021, 21, 5036-5049.	1.4	11
11727	Advancing solid-state band gap predictions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	3
11728	The structure and stability of faecal pigment-Zinc(II) complexes. <i>Journal of Molecular Structure</i> , 2021, 1238, 130440.	1.8	5
11729	Radical 1,4â€‘Aryl Migration Enabled Remote Crossâ€‘Electrophile Coupling of 1,2â€‘Bromo Acid Esters with Aryl Bromides. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 21360-21367.	7.2	22

#	ARTICLE	IF	CITATIONS
11730	Electrochemically modulated SERS detection of procaine using FTO electrodes modified with silver-decorated carbon nanosphere. <i>Electrochimica Acta</i> , 2021, 387, 138463.	2.6	33
11731	Short Excited-State Lifetimes Mediate Charge-Recombination Losses in Organic Solar Cell Blends with Low Charge-Transfer Driving Force. <i>Advanced Materials</i> , 2022, 34, e2101784.	11.1	11
11732	DFT Functionals for Modeling of Polyethylene Chains Cross-Linked by Metal Atoms. DLPNO-CCSD(T) Benchmark Calculations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7382-7395.	1.1	8
11733	Synthesis of Donor-Acceptor Conjugated Macrocycles by Post-Functionalization. <i>Chinese Journal of Chemistry</i> , 2021, 39, 2705-2710.	2.6	3
11734	Structural, elastic, vibrational, electronic and optical properties of SmFeO ₃ using density functional theory. <i>Physica B: Condensed Matter</i> , 2021, 615, 413061.	1.3	14
11735	Simulation of the electron ionization mass spectra of the Novichok nerve agent. <i>Journal of Mass Spectrometry</i> , 2021, 56, e4779.	0.7	5
11736	Machine Learning Directed Optimization of Classical Molecular Modeling Force Fields. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4400-4414.	2.5	29
11737	Growth and computational studies on vanillin isoniazid single crystals. <i>Chinese Journal of Physics</i> , 2021, 72, 229-239.	2.0	13
11738	Assessment of DFT methods for the prediction of detachment energies and electronic structures of complex and multiply charged anions. <i>Computational and Theoretical Chemistry</i> , 2021, 1202, 113295.	1.1	4
11739	Significant increase in dipole moments of functional groups using cation bonding for excellent SERS sensing as a universal approach. <i>Sensors and Actuators B: Chemical</i> , 2021, 340, 129960.	4.0	8
11740	Negatively charged polymeric interphase for regulated uniform lithium-ion transport in stable lithium metal batteries. <i>Nano Energy</i> , 2021, 87, 106214.	8.2	18
11741	A comparative study of structural, electronic, and optical properties of thiolated gold clusters with icosahedral vs face-centered cubic cores. <i>Journal of Chemical Physics</i> , 2021, 155, 094304.	1.2	4
11742	Stacked Ensemble Machine Learning for Range-Separation Parameters. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9516-9524.	2.1	9
11743	Synthesis of crown ether appended 25-Oxasamaragdyrins and their BF ₂ -Complexes. <i>Inorganica Chimica Acta</i> , 2021, 525, 120458.	1.2	1
11744	Metal Effect Meets Volcano Plots: A DFT Study on Tris(phosphino)borane-Transition Metal Complexes Catalyzed H ₂ Activation. <i>Chemistry - an Asian Journal</i> , 2021, 16, 3427-3436.	1.7	2
11745	Magnetic Aromaticity of Cycloporphyrin Nanorings. <i>Chemistry</i> , 2021, 3, 991-1004.	0.9	7
11746	Metal-Organic Frameworks of Magnesium Based on 2,5-Dihydroxy-3,6-di-tert-butyl-para-benzoquinone. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2021, 47, 610-619.	0.3	8
11747	Time-Resolved Spectroscopy and Electronic Structure of Mono- and Dinuclear Pyridyl-Triazole/DPEPhos-Based Cu(I) Complexes. <i>Chemistry - A European Journal</i> , 2021, 27, 15252-15271.	1.7	14

#	ARTICLE	IF	CITATIONS
11748	A self-consistent systematic optimisation of range-separated hybrid functionals from first principles. <i>Molecular Physics</i> , 0, , .	0.8	3
11749	Chemisorption of sulfaguanidine and sulfanilamide drugs on bismuthene nanosheet based on first-principles studies. <i>Applied Surface Science</i> , 2021, 561, 149990.	3.1	13
11750	Development of 1,3-diynyl derivatives of noscapine as potent tubulin binding anticancer agents for the management of breast cancer. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 13136-13153.	2.0	5
11751	Unified Mechanistic Concept of the Copper-Catalyzed and Amide-Oxazoline-Directed C(sp ²)-H Bond Functionalization. <i>ACS Catalysis</i> , 2021, 11, 12620-12631.	5.5	12
11752	Nonheme Iron Imido Complexes Bearing a Non-Innocent Ligand: A Synthetic Chameleon Species in Oxidation Reactions. <i>Chemistry - A European Journal</i> , 2021, 27, 17495-17503.	1.7	2
11754	Importance of the gas-phase error correction for O ₂ when using DFT to model the oxygen reduction and evolution reactions. <i>Journal of Electroanalytical Chemistry</i> , 2021, 896, 115178.	1.9	37
11755	Towards highly accurate calculations of parity violation in chiral molecules: relativistic coupled-cluster theory including QED-effects. <i>Molecular Physics</i> , 2021, 119, .	0.8	13
11756	Reactions of NO ₂ with aromatic aldehydes: gas-phase kinetics and insights into the mechanism of the reaction. <i>Atmospheric Chemistry and Physics</i> , 2021, 21, 13537-13551.	1.9	7
11757	Can the Antivirals Remdesivir and Favipiravir Work Better Jointly? In Silico Insights. <i>Drug Research</i> , 2022, 72, 34-40.	0.7	6
11758	Theoretical Studies via DFT Calculation of Pyrimidine Derivatives as Potential Corrosion Inhibitor. <i>Journal of the Institute of Science and Technology</i> , 0, , 2142-2151.	0.3	0
11759	New Hybrid (E)-4-(pyren-1-ylmethylene)amino-N-(thiazol-2-yl)benzenesulfonamide as a Potential Drug Candidate: Spectroscopy, TD-DFT, NBO, FMO, and MEP Studies**. <i>ChemistrySelect</i> , 2021, 6, 9369-9381.	0.7	13
11760	Synthesis and properties of covalently linked di-p-benzihomoporphyrin-BODIPY conjugates. <i>Journal of Porphyrins and Phthalocyanines</i> , 2021, 25, 1152-1160.	0.4	2
11761	On the Interactions of Melatonin/ β -Cyclodextrin Inclusion Complex: A Novel Approach Combining Efficient Semiempirical Extended Tight-Binding (xTB) Results with Ab Initio Methods. <i>Molecules</i> , 2021, 26, 5881.	1.7	16
11762	Synthesis of homo- and heterofunctionalized bay-annulated indigo derivatives and their properties. <i>Dyes and Pigments</i> , 2021, 193, 109535.	2.0	4
11763	A Convenient DFT-Based Strategy for Predicting Transition Temperatures of Valence Tautomeric Molecular Switches. <i>Inorganic Chemistry</i> , 2021, 60, 14475-14487.	1.9	14
11764	A member of p-type TCO family: Sn ₂ TaxNb _{2-x} O ₇ with a tunable band gap and controllable hole mobility. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 271, 115255.	1.7	0
11765	Synthesis and Properties of Symmetric Glycerol-Derived 1,2,3-Triethers and 1,3-Diether-2-Ketones for CO ₂ Absorption. <i>Chemical Engineering Science</i> , 2021, 248, 117150.	1.9	9
11766	Two-Dimensional Infrared Correlation Spectroscopy, Conductor-like Screening Model for Real Solvents, and Density Functional Theory Study on the Adsorption Mechanism of Polyvinylpyrrolidone for Effective Phenol Removal in an Aqueous Medium. <i>ACS Omega</i> , 2021, 6, 25179-25192.	1.6	8

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11767	Origin-Independent Densities of Static and Dynamic Molecular Polarizabilities. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8855-8864.	2.1	5
11768	Machine-Learning-Assisted Free Energy Simulation of Solution-Phase and Enzyme Reactions. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5745-5758.	2.3	55
11769	A Joint Venture of Ab Initio Molecular Dynamics, Coupled Cluster Electronic Structure Methods, and Liquid-State Theory to Compute Accurate Isotropic Hyperfine Constants of Nitroxide Probes in Water. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6366-6386.	2.3	11
11771	Design, synthesis and biological evaluation of novel thiohydantoin derivatives as antiproliferative agents: A combined experimental and theoretical assessments. <i>Journal of Molecular Structure</i> , 2022, 1249, 131574.	1.8	13
11772	Synthesis, Crystal structure, Hirshfeld surface analysis, Spectral characterizations and Quantum computational assessments of 1-hydroxy-3-methyl-1H-pyrido[2,1-b]quinazolin-11-one. <i>Journal of Molecular Structure</i> , 2021, , 131592.	1.8	5
11773	GW approximation for open-shell molecules: a first-principles study. <i>New Journal of Physics</i> , 2021, 23, 093027.	1.2	5
11774	Investigating Tetrel-Based Neutral Frustrated Lewis Pairs for Hydrogen Activation. <i>Inorganic Chemistry</i> , 2021, 60, 15180-15189.	1.9	9
11775	Optimizing the Cosensitization Effect of SQ02 Dye on BP-2 Dye-Sensitized Solar Cells: A Computational Quantum Chemical Study. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5098-5116.	2.5	16
11776	Degradation of polybenzimidazole in alkaline solution with first-principles Modeling. <i>Electrochimica Acta</i> , 2021, 398, 139329.	2.6	5
11777	Electronic properties and reactivity patterns of d^0 species of Mn, Fe, Co, and Ni. <i>Bulletin of the Korean Chemical Society</i> , 2021, 42, 1506-1512.	1.0	9
11778	Insights into unexpected photoisomerization from photooxidation of tribromoacetic acid in aqueous environment using ultrafast spectroscopy. <i>Journal of Hazardous Materials</i> , 2021, 418, 126214.	6.5	1
11779	Synthesis of Cationic Silaamidinate Germylenes and Stannylenes and the Catalytic Application for Hydroboration of Pyridines. <i>Inorganic Chemistry</i> , 2021, 60, 14038-14046.	1.9	7
11780	Zipper phosphorene as sensing element towards formaldehyde and acetaldehyde – A first-principles insight. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 107, 107971.	1.3	19
11781	Accurate Prediction of Band Structure of FeS ₂ : A Hard Quest of Advanced First-Principles Approaches. <i>Frontiers in Chemistry</i> , 2021, 9, 747972.	1.8	1
11782	New insights into colloidal GO, Cr(VI) and Fe(II) interaction by a combined batch, spectroscopic and DFT calculation investigation. <i>Journal of Molecular Liquids</i> , 2021, 337, 116365.	2.3	13
11783	Benchmark test of a dispersion corrected revised Tao-Mo semilocal functional for thermochemistry, kinetics, and noncovalent interactions of molecules and solids. <i>Journal of Chemical Physics</i> , 2021, 155, 114102.	1.2	4
11784	A crossed molecular beam investigation of the N(2D) ⁺ -pyridine reaction and implications for prebiotic chemistry. <i>Chemical Physics Letters</i> , 2021, 779, 138852.	1.2	12
11785	Fabrication, DFT modeling, and photoelectronic characterizations of novel pyridinylcarbonylquinoline for promising potential energy conversion. <i>Journal of Materials Research and Technology</i> , 2021, 14, 3092-3110.	2.6	5

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11787	Intramolecular Charge Transfer in the Azathioprine Prodrug Quenches Intersystem Crossing to the Reactive Triplet State in 6-Mercaptopurine. <i>Photochemistry and Photobiology</i> , 2022, 98, 617-632.	1.3	3
11788	Spatial Contributions to ¹ H NMR Chemical Shifts of Free-Base Porphyrinoids. <i>Chemistry</i> , 2021, 3, 1005-1021.	0.9	6
11789	Solvation Structure around Li ⁺ Ions in Organic Carbonate Electrolytes: Spacer-Free Thin Cell IR Spectroscopy. <i>Analytical Chemistry</i> , 2021, 93, 12594-12601.	3.2	13
11790	A Theoretical Insight of Cr Dopant in Tungsten Oxide for Gas Sensor Application. <i>Materials Today Communications</i> , 2021, 28, 102508.	0.9	6
11791	A black-box, general purpose quadratic self-consistent field code with and without Cholesky decomposition of the two-electron integrals. <i>Molecular Physics</i> , 2021, 119, .	0.8	8
11792	Switching of second-order nonlinear response effected by different acceptors: The impacts of environment and frequency dispersion. <i>Dyes and Pigments</i> , 2021, 193, 109502.	2.0	7
11793	Structural, surface, and computational analysis of two vitamin-B1 crystals with sulfonimide-based anions. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2021, .	0.4	0
11794	Synthesis, Computational, Antibacterial and Antifungal Investigation of Two Tri-Fluorinated Chalcones of 1-(2,3-Dihydrobenzo[<i>b</i>][1,4]dioxin-6-yl)ethan-1-one. <i>Polycyclic Aromatic Compounds</i> , 2022, 42, 6155-6172.	1.4	7
11795	DFT-Machine Learning Approach for Accurate Prediction of ρ . <i>Journal of Physical Chemistry A</i> , 2021, 125, 8712-8722.	1.1	15
11796	A Comprehensive Review on the Applications of Boron Nitride Nanomaterials in Membrane Fabrication and Modification. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 13391-13424.	1.8	35
11797	Synthesis of Mono β -Pyrrole Substituted Triphyrin(2.1.1)s. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 3297-3307.	1.3	3
11798	A Two-Step Baromechanical Cycle for Repeated Activation and Deactivation of Mechanophores. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9470-9474.	2.1	5
11799	Nonlinear optical behavior of non-centrosymmetric biferrocenyl Schiff-base derivatives and their DNA binding potential supported by DFT and electrochemical investigations. <i>Applied Organometallic Chemistry</i> , 2021, 35, e6449.	1.7	0
11800	Highly selective adsorption of SO ₂ on WX ₂ (X = S, Se, Te) monolayers and the effect of strain engineering: a DFT study. <i>Journal of Computational Electronics</i> , 2021, 20, 1874-1883.	1.3	1
11801	Noncovalent Interactions in Organic Radicals: Pancake, π -Hole, and H-Bonding in F2HbimDTDA. <i>Crystal Growth and Design</i> , 0, .	1.4	2
11802	Self-assembled monolayers of oligophenylenes stiffer than steel and silicon, possibly even stiffer than Si ₃ N ₄ . <i>Applied Surface Science Advances</i> , 2021, 5, 100094.	2.9	1
11803	Nonadiabatic dynamics with spin-flip vs linear-response time-dependent density functional theory: A case study for the protonated Schiff-base C ₅ H ₆ NH ₂ ⁺ . <i>Journal of Chemical Physics</i> , 2021, 155, 124111.	1.2	14
11804	Rise of silicene and its applications in gas sensing. <i>Journal of Molecular Modeling</i> , 2021, 27, 277.	0.8	11

#	ARTICLE	IF	CITATIONS
11823	Highly Efficient Microwave-Assisted Solvent Free Sequential One-Pot Multicomponent Synthesis of Novel 2- α -Hydroxy Indenopyridin-5-ones and Mechanistic Computational Study. <i>Journal of Heterocyclic Chemistry</i> , 0, , .	1.4	0
11824	Synthesis of three quasi liquid Schiff bases between hexanal and adenine, cytosine, and l-leucine, structural interpretation, quantum mechanical studies and biological activity prediction. <i>Journal of Molecular Liquids</i> , 2021, 341, 117305.	2.3	22
11825	A rotational study of the 1:1 adduct of ethanol and 1,4-dioxane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 261, 120086.	2.0	2
11826	Realizing wide-temperature Zn metal anodes through concurrent interface stability regulation and solvation structure modulation. <i>Energy Storage Materials</i> , 2021, 42, 517-525.	9.5	47
11827	Hybrid exchange-correlation energy functionals for accurate prediction of the electronic and optical properties of alkaline-earth metal oxides. <i>Materials Science in Semiconductor Processing</i> , 2021, 135, 106092.	1.9	6
11828	Structural and spectroscopic analysis of the Cis-Trans isomers of the captopril in the gaseous and aqueous phases. <i>Journal of Molecular Structure</i> , 2021, 1243, 130872.	1.8	2
11829	Spin-state energetics of manganese spin crossover complexes: Comparison of single-reference and multi-reference ab initio approaches. <i>Polyhedron</i> , 2021, 208, 115399.	1.0	14
11830	Tailoring, structural elucidation, DFT calculation, DNA interaction and pharmaceutical applications of some aryl hydrazone Mn(II), Cu(II) and Fe(III) complexes. <i>Journal of Molecular Structure</i> , 2021, 1244, 131017.	1.8	66
11831	(-)-Tubifolidine as strychnos indole alkaloid: Spectroscopic characterization (FT-IR, NMR, UV-Vis), antioxidant activity, molecular docking, and DFT studies. <i>Journal of Molecular Structure</i> , 2021, 1244, 130978.	1.8	16
11832	Synthesis, spectra (FT-IR, NMR) investigations, DFT study, in silico ADMET and Molecular docking analysis of 2-amino-4-(4-aminophenyl)thiophene-3-carbonitrile as a potential anti-tubercular agent. <i>Journal of Molecular Structure</i> , 2021, 1244, 130880.	1.8	53
11833	Sulphido bridged dinuclear quadruple bond cleavage product from the reaction between $\text{Re}_2(\mu\text{-O}_2\text{CCH}_3)_4\text{Cl}_2$ and dithiocarbamate: An experimental and theoretical study. <i>Polyhedron</i> , 2021, 208, 115422.	1.0	0
11834	Optical and NLO properties of zigzag carbon nanobelt compounds. <i>Journal of Molecular Structure</i> , 2021, 1244, 130936.	1.8	2
11835	Synthesis, spectroscopic characterization, DFT calculations, and molecular docking studies of new unsymmetric bishydrazone derivatives. <i>Journal of Molecular Structure</i> , 2021, 1244, 131224.	1.8	13
11836	Molecular structure, tautomer's, reactivity and inhibition studies on 6-Methyl-2-thiouracil for mild steel corrosion in aqueous HCl (1.00 M): Experimental and Theoretical Studies. <i>Journal of Molecular Structure</i> , 2021, 1244, 130927.	1.8	31
11837	Multiscale modeling of ZnO nanoparticle synthesis: Chemical kinetics and Turing instability. <i>Materials Today Communications</i> , 2021, 29, 102748.	0.9	3
11838	Synthesis, spectroscopic characterization, molecular docking studies and DFT calculation of novel Mannich base 1-((4-ethylpiperazin-1-yl)(2-hydroxyphenyl)methyl)naphthalen-2-ol. <i>Journal of Molecular Structure</i> , 2021, 1246, 131164.	1.8	31
11839	Implications for the Nb aggregation inherited from melt to $\hat{\Gamma}^3$ phase of U-Nb alloy. <i>Journal of Alloys and Compounds</i> , 2021, 885, 160537.	2.8	0
11840	Fast and sensitive detection of Procainamide: Combined SERS and DFT modeling studies. <i>Journal of Molecular Liquids</i> , 2021, 343, 117633.	2.3	23

#	ARTICLE	IF	CITATIONS
11841	Theoretical studies of dimers and properties of the corrosion inhibitor profile for semicarbazones and thiosemicarbazones. <i>Journal of Molecular Liquids</i> , 2021, 343, 117660.	2.3	6
11842	Adsorption behaviour of sulfoxazole molecules on tricycle arsenene nanoribbon - a first-principles study. <i>Journal of Molecular Liquids</i> , 2021, 343, 117635.	2.3	21
11843	Experimental and DFT investigation on N-functionalized biochars for enhanced removal of Cr(VI). <i>Environmental Pollution</i> , 2021, 291, 118244.	3.7	15
11844	Improved NH ₃ -N conversion efficiency to N ₂ activated by BDD substrate on NiCu electrocatalysis process. <i>Separation and Purification Technology</i> , 2021, 276, 119350.	3.9	12
11845	Solution-processed Cd-substituted CZTS nanocrystals for sensitized liquid junction solar cells. <i>Journal of Alloys and Compounds</i> , 2022, 890, 161575.	2.8	9
11846	An efficient studies on C-2 cyanomethylation of the indole synthesis: The electronic and spectroscopic characterization (FT-IR, NMR, UV-Vis), antioxidant activity, and theoretical calculations. <i>Journal of Molecular Structure</i> , 2022, 1247, 131416.	1.8	8
11847	Electronic transport via DTF-NEGF at bipyridine junctions with 1D organic electrodes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 135, 114953.	1.3	0
11848	Synthesis, crystal structures, optical properties, DFT and TD-DFT studies of Ni (II) complexes with imine-based ligands. <i>Journal of Molecular Structure</i> , 2022, 1247, 131351.	1.8	7
11849	Synthesis, crystal structure, Hirshfeld surface analysis and DFT calculations of 2, 2, 2-tribromo-1-(3,5-dibromo-2-hydroxyphenyl)ethanone. <i>Journal of Molecular Structure</i> , 2022, 1248, 131313.	1.8	2
11850	[Diaquo{bis(p-hydroxybenzoato- λ^1 O1)}(1-methylimidazole- λ^1 N1)}copper(II)]: Synthesis, crystal structure, catalytic activity and DFT study. <i>Journal of Molecular Structure</i> , 2022, 1247, 131323.	1.8	3
11851	SCXRD, DFT and molecular docking based structural analyses towards novel 3-piperazin-1-yl-benzo[d]isothiazole and 3-piperidin-4-yl-benzo[d]isoxazoles appended to quinoline as pharmacological agents. <i>Journal of Molecular Structure</i> , 2022, 1248, 131442.	1.8	4
11852	A density functional theory study on favipiravir drug interaction with BN-doped C60 heterofullerene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 135, 114950.	1.3	22
11853	Rapid atmospheric carbon dioxide fixation by nickel($\langle \text{sc} \rangle \text{ii} \langle \text{sc} \rangle$) complexes: meridionally coordinated diazepane-based 3N ligands facilitate fixation. <i>Dalton Transactions</i> , 2021, 50, 8045-8056.	1.6	3
11854	Feasibility of Predicting Static Dielectric Constants of Polymer Materials: A Density Functional Theory Method. <i>Polymers</i> , 2021, 13, 284.	2.0	14
11855	Photocatalytic degradation of acetaminophen and caffeine using magnetite-hematite combined nanoparticles: kinetics and mechanisms. <i>Environmental Science and Pollution Research</i> , 2021, 28, 17228-17243.	2.7	15
11856	Contact residue contributions to interaction energies between SARS-CoV-1 spike proteins and human ACE2 receptors. <i>Scientific Reports</i> , 2021, 11, 1156.	1.6	6
11857	Identifying the preferential pathways of CO ₂ capture and hydrogenation to methanol over an Mn($\langle \text{sc} \rangle \text{i} \langle \text{sc} \rangle$)â€“PNP catalyst: a computational study. <i>Dalton Transactions</i> , 2021, 50, 9598-9609.	1.6	5
11858	Pyran based bipodal Dâ€“iâ€“A systems: colorimetric and ratiometric sensing of mercury â€“ experimental and theoretical approach. <i>New Journal of Chemistry</i> , 2021, 45, 15780-15788.	1.4	1

#	ARTICLE	IF	CITATIONS
11859	Laboratory Observation of, Astrochemical Search for, and Structure of Elusive Erythrulose in the Interstellar Medium. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1352-1359.	2.1	6
11860	Oligoene and cyanine features of tetracyano quinoidal oligothiophenes. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10727-10740.	2.7	6
11861	Quantifying Uncertainties in Solvation Procedures for Modeling Aqueous Phase Reaction Mechanisms. <i>Journal of Physical Chemistry A</i> , 2021, 125, 154-164.	1.1	24
11862	Forecasting System of Computational Time of DFT/TDDFT Calculations under the Multiverse Ansatz via Machine Learning and Cheminformatics. <i>ACS Omega</i> , 2021, 6, 2001-2024.	1.6	6
11863	Stabilization of uranyl(UO_2^{2+}) by dipicolinic acid in aqueous medium. <i>Dalton Transactions</i> , 2021, 50, 1486-1495.	1.6	11
11864	Valence tautomeric transformation in the [CrCo] compound: exploration of cooperative interactions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21714-21728.	1.3	1
11865	An efficient implementation of spin-orbit coupling within the framework of semiempirical orthogonalization-corrected methods for ultrafast intersystem crossing dynamics. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22313-22323.	1.3	4
11866	Crystallographic, spectroscopic, thermal, optical investigations and density functional theory calculations for novel Co(II) and Mn(II) complexes. <i>Applied Physics A: Materials Science and Processing</i> , 2021, 127, 1.	1.1	11
11867	Mechanochromism and Aggregation-Induced Emission in Phenanthroimidazole Derivatives: Role of Positional Change of Different Donors in a Multichromophoric Assembly. <i>Journal of Organic Chemistry</i> , 2021, 86, 1560-1574.	1.7	55
11868	Computational modelling of Pd-catalysed alkoxy carbonylation of alkenes and alkynes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15869-15880.	1.3	7
11869	Antioxidant activity of the hazelnut plant determination by computational chemistry methods. <i>Main Group Chemistry</i> , 2021, 19, 273-282.	0.4	2
11870	Hydrothermal synthesis of biocompatible nitrogen doped graphene quantum dots. <i>Energy and Environment</i> , 2021, 32, 1170-1182.	2.7	11
11871	Quantum-chemical study of octafluoro- $\text{C}_{22}\text{H}_2\text{F}_{18}$ spiropi[triphosphazene]. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26613.	1.0	0
11872	Folding and fluorescence enhancement with strong odd-even effect for a series of merocyanine dye oligomers. <i>Chemical Science</i> , 2021, 12, 8342-8352.	3.7	21
11873	On the origins of the mechanistic variants in the thermal reactions of S_{2n+1} ($n = 1-3$) with benzene. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17512-17520.	1.3	4
11874	Measurement of the conformational switching of azobenzenes from the macro- to attomolar scale in self-assembled 2D and 3D nanostructures. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11698-11708.	1.3	3
11875	Aromaticity in molecules and transition structures: from atomic and molecular orbitals to simple ring current models. , 2021, , 1-41.		0
11876	Influence of molybdenum and technetium doping on visible light absorption, optical and electronic properties of lead-free perovskite CsSnBr_3 for optoelectronic applications. <i>RSC Advances</i> , 2021, 11, 2405-2414.	1.7	23

#	ARTICLE	IF	CITATIONS
11877	Probing reaction processes and reversibility in Earth-abundant Na ₃ FeF ₆ for Na-ion batteries. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20052-20064.	1.3	5
11878	Are all charge-transfer parameters created equally? A study of functional dependence and excited-state charge-transfer quantification across two dye families. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20583-20597.	1.3	3
11879	The photophysical properties of naphthalene bridged disilanes. <i>RSC Advances</i> , 2021, 11, 21343-21350.	1.7	1
11880	A paper-based colorimetric chemosensor for rapid and highly sensitive detection of sulfide for environmental monitoring. <i>Analytical Methods</i> , 2021, 13, 1332-1339.	1.3	20
11881	The substituent effect on chemical reactivity of (9H-pyrido[3,4-b]indole-3-yl)methanol: Spectroscopic and electronic investigation. <i>Materials Today: Proceedings</i> , 2021, 45, 7370-7376.	0.9	0
11882	Towards correlating dimensionality and topology in luminescent MOFs based on terephthalato and bispyridyl-like ligands. <i>Dalton Transactions</i> , 2021, 50, 9269-9282.	1.6	5
11883	Determining electron-nucleus distances and Fermi contact couplings from ENDOR spectra. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8326-8335.	1.3	5
11884	Corrole-Substituted Fluorescent Heme Proteins. <i>Inorganic Chemistry</i> , 2021, 60, 2716-2729.	1.9	17
11885	Rationalization of the mechanism and chemoselectivity of versatile Au-catalyzed reactions of diazoesters with allyl-functionalized sulfides, selenides, amines, or ethers by DFT. <i>Organic Chemistry Frontiers</i> , 2021, 8, 6053-6062.	2.3	3
11886	Metal-free photocatalytic aerobic oxidation of biomass-based furfural derivatives to prepare β -butyrolactone. <i>Green Chemistry</i> , 2021, 23, 1758-1765.	4.6	13
11887	How Beneficial Is the Explicit Account of Doubly-Excited Configurations in Linear Response Theory?. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 975-984.	2.3	12
11888	Computational insights into Ir-catalyzed allylic C-H amination of terminal alkenes: mechanism, regioselectivity, and catalytic activity. <i>RSC Advances</i> , 2021, 11, 19113-19120.	1.7	2
11889	Fluorescent chemosensors for Hg ²⁺ ions based on a pyridine-attached phenanthridine probe. <i>New Journal of Chemistry</i> , 2021, 45, 17667-17673.	1.4	5
11890	Organotin Schiff bases as halofluorochromic dyes: green synthesis, chemio-photophysical characterization, DFT, and their fluorescent bioimaging <i>in vitro</i> . <i>Journal of Materials Chemistry B</i> , 2021, 9, 7698-7712.	2.9	12
11895	Organocatalytic Enantioselective Higher-Order Cycloadditions of In Situ Generated Amino Isobenzofulvenes. <i>Angewandte Chemie</i> , 2018, 130, 1260-1264.	1.6	16
11896	An efficient method to prepare sulfoxonium ylides and their reactivity studies using copper powder and Sc(III) as catalysts: Molecular and electronic structure analysis. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5748.	1.7	10
11897	Parallel Versus Antiparallel β -Sheet Structure in Cyclic Peptide Hybrids Containing β - or α -Cyclic Amino Acids. <i>Chemistry - A European Journal</i> , 2020, 26, 5846-5858.	1.7	12
11898	Electron-Rich Phenothiazine Congeners and Beyond: Synthesis and Electronic Properties of Isomeric Dithieno[1,4]thiazines. <i>Chemistry - A European Journal</i> , 2020, 26, 12111-12118.	1.7	15

#	ARTICLE	IF	CITATIONS
11899	Synthesis, Characterization and Biological Potency of Butylâ€Pyridone Based Azo Dyes. ChemistrySelect, 2020, 5, 5460-5464.	0.7	8
11900	W1 and W2 Theories, and Their Variants: Thermochemistry in the kJ/mol Accuracy Range. , 2001, , 31-65.		25
11901	Theoretical Prediction of Bond Dissociation Energies for Transition Metal Compounds and Main Group Complexes with Standard Quantum-Chemical Methods. , 2001, , 199-233.		4
11902	Hohenberg-Kohn-Sham Density Functional Theory. Challenges and Advances in Computational Chemistry and Physics, 2007, , 153-201.	0.6	1
11903	Localization via Density Functionals. Topics in Current Chemistry, 1999, , 201-230.	4.0	1
11904	Analysis and modelling of atomic and molecular kohn-sham potentials. Topics in Current Chemistry, 1996, , 107-167.	4.0	31
11905	A Critical Assessment of Density Functional Theory with Regard to Applications in Organometallic Chemistry. Topics in Organometallic Chemistry, 1999, , 109-163.	0.7	59
11906	Thomas-Fermi and Other Density-Functional Theories. , 2006, , 295-306.		4
11907	Nanoscale Atomic Clusters, Complexity of. , 2009, , 5889-5912.		4
11908	The Oniom Method and its Applications to Enzymatic Reactions. Challenges and Advances in Computational Chemistry and Physics, 2009, , 21-55.	0.6	15
11909	The Pair Density in Approximate Density Functionals: The Hidden Agent. Mathematical and Computational Chemistry, 2000, , 183-208.	0.3	3
11910	Density Functional Theory for The Study of Single-Molecule Electronic Systems. , 1999, , 439-450.		3
11911	Density Functional and Neural Network Analysis. , 1997, , 255-277.		13
11912	Mixing Exact Exchange with GGA: When to Say When. , 1998, , 57-68.		32
11913	Adiabatic Coupling in the Helium and the Beryllium Series. , 1998, , 69-80.		4
11914	A Theoretical Investigation of the Reactions of N(2D) with Small Alkynes and Implications for the Prebiotic Chemistry of Titan. Lecture Notes in Computer Science, 2020, , 717-729.	1.0	3
11915	A Theoretical Study on a Visible-Light Photo-Catalytic Activity in Carbon-Doped SrTiO3 Perovskite. Progress in Theoretical Chemistry and Physics, 2013, , 221-232.	0.2	3
11916	A Theoretical Study on Proton Conduction Mechanism in BaZrO3 Perovskite. Progress in Theoretical Chemistry and Physics, 2013, , 233-248.	0.2	8

#	ARTICLE	IF	CITATIONS
11917	Ab-Initio and DFT Study of the Muchimangin-B Molecule. Progress in Theoretical Chemistry and Physics, 2015, , 91-114.	0.2	1
11918	Small Polarons in Transition Metal Oxides. , 2020, , 1035-1073.		10
11919	Review on Simulation Models for Materials and Biomolecular Study and Design. , 2017, , 373-408.		3
11920	Fundamentals of Infrared and Raman Spectroscopy, SERS, and Theoretical Simulations. , 2008, , 9-35.		4
11921	A New Generation of Doubly Hybrid Density Functionals (DHDFs). Springer Briefs in Molecular Science, 2014, , 25-45.	0.1	2
11922	Ab initio quantum chemical and ReaxFF-based study of the intramolecular iminiumâ€“enamine conversion in a proline-catalyzed reaction. Highlights in Theoretical Chemistry, 2014, , 205-215.	0.0	1
11923	Perspective on â€œDensity functional thermochemistry. III. The role of exact exchangeâ€“, 2000, , 361-363.		29
11924	Potential Energy Surfaces for Reaction Catalyzed by Metalloenzymes from Quantum Chemical Computations. NATO Science for Peace and Security Series A: Chemistry and Biology, 2009, , 275-313.	0.5	1
11925	Methods for Hartree-Fock and Density Functional Theory Electronic Structure Calculations with Linearly Scaling Processor Time and Memory Usage. Challenges and Advances in Computational Chemistry and Physics, 2011, , 263-300.	0.6	6
11926	Description of Core-Ionized and Core-Excited States by Density Functional Theory and Time-Dependent Density Functional Theory. Progress in Theoretical Chemistry and Physics, 2012, , 275-308.	0.2	2
11927	Weak Intermolecular Interactions: A Supermolecular Approach. , 2015, , 1-27.		4
11928	Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2015, , 1-67.		5
11929	The Origin of the Molecular Atomization Energy Explained with the HF and HF-CC Models. , 2003, , 601-629.		4
11930	Ab Initio Simulation of Cu-Species in Zeolites: Siting, Coordination, UV-Vis Spectra and Reactivity. , 2001, , 221-234.		6
11932	Quantum Chemical Studies of Transition Metal Catalyzed Enzyme Reactions. , 1997, , 233-253.		4
11933	Extending the Marcus λ -Scale of Solvent Softness Using Conceptual Density Functional Theory and the Orbital Overlap Distance: Method and Application to Ionic Liquids. Journal of Solution Chemistry, 2020, 49, 614-628.	0.6	2
11934	Reactivity and Catalysis by Nanoalloys. , 2020, , 267-345.		2
11935	Use of dual-filtering to create training sets leading to improved accuracy in quantitative structure-retention relationships modelling for hydrophilic interaction liquid chromatographic systems. Journal of Chromatography A, 2017, 1507, 53-62.	1.8	26

#	ARTICLE	IF	CITATIONS
11936	Use of a theoretical prediction method and quantum chemical calculations for the design, synthesis and experimental evaluation of three green corrosion inhibitors for mild steel. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 599, 124857.	2.3	28
11937	Low-energy-gap organic photosensitizers with phenalenothiophene and benzoindeno[1,2-b]thiophene as primary electron-donors for durable dye-sensitized solar cells. <i>Journal of Power Sources</i> , 2020, 451, 227748.	4.0	12
11938	Straight Z and twisted E isomers from triphenylamine derivatives: Intramolecular charge transfer and second-order nonlinear optical response. <i>Journal of Molecular Liquids</i> , 2020, 311, 113297.	2.3	9
11939	Study the solvation effect on 6-phenyl-2-thioxo-1,2-dihydropyridine-3-carbonitrile derivatives by TD-DFT calculations and molecular dynamics simulations. <i>Journal of Molecular Structure</i> , 2020, 1200, 127056.	1.8	16
11940	Arsenic pentafluoride surface adsorption studies on Kagome-phosphorene – a DFT outlook. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126552.	0.9	16
11941	Vibrational Spectroscopic Studies of Nitrated Polycyclic Aromatic Hydrocarbons (NPAHs): A Review (1960-2019). <i>Vibrational Spectroscopy</i> , 2020, 109, 103072.	1.2	4
11942	How similar are HF, MP2, and DFT charge distributions in the Cr(CO) ₆ complex?. <i>Advances in Molecular Similarity</i> , 1996, , 167-186.	0.5	2
11943	Optimizing hybrid density functionals by means of quantum molecular similarity techniques. <i>Advances in Molecular Similarity</i> , 1999, , 187-203.	0.5	2
11945	Insights into the Chemical Reactivity in Acetyl-CoA Synthase. <i>Inorganic Chemistry</i> , 2020, 59, 15167-15179.	1.9	11
11946	<i>Ab Initio</i> Molecular Dynamics Investigation of Beryllium Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 2413-2425.	1.9	7
11947	Energy Landscapes for Electronic Structure. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 151-169.	2.3	18
11948	Stereoselective Reductions of 3-Substituted Cyclobutanones: A Comparison between Experiment and Theory. <i>Journal of Organic Chemistry</i> , 2020, 85, 7803-7816.	1.7	5
11950	Lactic Acid Spectroscopy: Intra- and Intermolecular Interactions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 218-229.	1.1	7
11951	The Elusive Noncanonical Isomers of Ionized 9-Methyladenine and 2-Deoxyadenosine. <i>Journal of Physical Chemistry A</i> , 2021, 125, 338-348.	1.1	6
11952	Accurate Assignments of Excited-State Resonance Raman Spectra: A Benchmark Study Combining Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7937-7946.	1.1	26
11953	Band Gap Narrowing of Bi-Doped NaTaO ₃ for Photocatalytic Hydrogen Evolution under Simulated Sunlight: A Pseudocubic Phase Induced by Doping. <i>ACS Applied Energy Materials</i> , 2021, 4, 671-679.	2.5	21
11954	$\hat{\rho}^2$ -(Z) Selectivity Control by Cyclometalated Rhodium(III)-Triazolylidene Homogeneous and Heterogeneous Terminal Alkyne Hydrosilylation Catalysts. <i>ACS Catalysis</i> , 2020, 10, 13334-13351.	5.5	28
11955	Theoretical and physical aspects of nuclear shielding. <i>Nuclear Magnetic Resonance</i> , 2012, , 38-55.	0.1	3

#	ARTICLE	IF	CITATIONS
11956	Isomerization versus dissociation of phenylalanylglycyltryptophan radical cations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16923-16933.	1.3	1
11957	Polyaniline and CN-functionalized polyaniline as organic cathodes for lithium and sodium ion batteries: a combined molecular dynamics and density functional tight binding study in solid state. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 232-237.	1.3	27
11958	Self-assembled cobalt(<i>scp</i>)porphyrinâ€‘fulleropyrrolidine triads <i>via</i> axial coordination with photoinduced electron transfer. <i>New Journal of Chemistry</i> , 2018, 42, 12449-12456.	1.4	31
11959	Effects of incorporating regioisomers and flexible rotors to direct aggregation induced emission to achieve stimuli-responsive luminogens, security inks and chemical warfare agent sensors. <i>Chemical Communications</i> , 2020, 56, 7633-7636.	2.2	21
11960	Understanding the structures and aromaticity of heteroporphyrins with computations. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 4415-4422.	1.5	7
11961	Allyl amino-thioxanthone derivatives as highly efficient visible light H-donors and co-polymerizable photoinitiators. <i>Polymer Chemistry</i> , 2020, 11, 4297-4312.	1.9	28
11962	Effects of Cr- and Mn-alloying on the band gap tuning, and optical and electronic properties of lead-free CsSnBr ₃ perovskites for optoelectronic applications. <i>RSC Advances</i> , 2020, 10, 43660-43669.	1.7	26
11963	Substituent effects on the O-H bond dissociation enthalpies in phenolic compounds: agreements and controversies. <i>Pure and Applied Chemistry</i> , 1999, 71, 1249-1256.	0.9	58
11964	Probing the interaction of (001) carbonated hydroxylapatite surfaces with water: a density functional investigation. <i>Micro and Nano Letters</i> , 2018, 13, 4-8.	0.6	11
11965	ALMA chemical survey of disk-outflow sources in Taurus (ALMA-DOT). <i>Astronomy and Astrophysics</i> , 2020, 644, A120.	2.1	10
11966	Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response. <i>Journal of Chemical Physics</i> , 2020, 152, 044111.	1.2	22
11967	Nonlocal rung-3.5 correlation from the density matrix expansion: Flat-plane condition, thermochemistry, and kinetics. <i>Journal of Chemical Physics</i> , 2020, 153, 164116.	1.2	3
11968	Large coupling-strength expansion of the MÃ‘llerâ€‘Plesset adiabatic connection: From paradigmatic cases to variational expressions for the leading terms. <i>Journal of Chemical Physics</i> , 2020, 153, 214112.	1.2	16
11969	A Sesquiterpene Isonitrile with a New Tricyclic Skeleton from the Indo-Pacific Nudibranch <i>Phyllidiella pustulosa</i> : Spectroscopic and Computational Studies. <i>Australian Journal of Chemistry</i> , 2020, 73, 129.	0.5	9
11970	Quasirelativistic two-component core excitations and polarisabilities from a damped-response formulation of the Betheâ€‘Salpeter equation. <i>Molecular Physics</i> , 2020, 118, e1755064.	0.8	38
11971	Correlation matrix renormalization theory in multi-band lattice systems. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 095902.	0.7	3
11973	Accuracy of electron densities obtained via Koopmans-compliant hybrid functionals. <i>Physical Review Materials</i> , 2018, 2, .	0.9	18
11974	Thermal expansion in dispersion-bound molecular crystals. <i>Physical Review Materials</i> , 2018, 2, .	0.9	18

#	ARTICLE	IF	CITATIONS
11975	Non-Heisenberg covalent magnetism in iron oxide clusters. Physical Review Materials, 2018, 2, .	0.9	6
11976	Hole-induced electronic and optical transitions in $\text{Li}_a\text{S}_r\text{Fe}_x\text{M}_y$	0.9	33
11977	Nonlocal van der Waals functionals for solids: Choosing an appropriate one. Physical Review Materials, 2019, 3, .	0.9	65
11978	Dielectric-dependent hybrid functionals for heterogeneous materials. Physical Review Materials, 2019, 3, .	0.9	36
11979	Nonempirical hybrid functionals for band gaps of inorganic metal-halide perovskites. Physical Review Materials, 2019, 3, .	0.9	35
11980	Vibrational mode contribution to the dielectric permittivity of disordered small-molecule organic semiconductors. Physical Review Materials, 2020, 4, .	0.9	8
11981	Interfacial electronic states of misfit heterostructure between hexagonal ZnO and cubic NiO. Physical Review Materials, 2020, 4, .	0.9	5
11982	Density functionals and Kohn-Sham potentials with minimal wavefunction preparations on a quantum computer. Physical Review Research, 2020, 2, .	1.3	4
11983	Charge densities in actinide compounds: strategies for data reduction and model building. IUCr, 2019, 6, 895-908.	1.0	7
11984	Morphology of the GdVO_4 crystal: first-principles studies. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 749-756.	0.5	4
11985	Franck-Condon Dominated Chemistry. Formation and Dissociations of the Dimethylhydroxysulfuranyl Radical. Collection of Czechoslovak Chemical Communications, 2000, 65, 455-476.	1.0	21
11986	A Combined ab initio and Density Functional Study of the Electronic Structure of Thymine and 2-Thiothymine Radicals. Collection of Czechoslovak Chemical Communications, 2003, 68, 2322-2334.	1.0	1
11987	2-Deoxyribose Radicals in the Gas Phase and Aqueous Solution. Transient Intermediates of Hydrogen Atom Abstraction from 2-Deoxyribofuranose. Collection of Czechoslovak Chemical Communications, 2005, 70, 1769-1786.	1.0	5
11988	NEW SORBENTS FOR DESULFURIZATION OF TRANSPORTATION FUELS. , 2003, , .		2
11989	Corrosion Inhibition of Mild Steel by newly Synthesized Pyrazole Carboxamide Derivatives in HCl Acid Medium: Experimental and Theoretical Studies. Journal of the Electrochemical Society, 2020, 167, 155508.	1.3	43
11990	A comprehensive analysis of the history of DFT based on the bibliometric method RPYS. Journal of Cheminformatics, 2019, 11, 72.	2.8	22
11991	Vibrational Circular Dichroism Spectroscopy. , 2003, , .		2
11992	Density-Functional Theory. , 2003, , .		8

#	ARTICLE	IF	CITATIONS
11993	Fundamental Concepts in Molecular Simulation of NO _x Catalysis. , 2005, , 233-268.		5
11994	Role of the Propionic Acid Side-Chain of C-Phycocyanin Chromophores in the Excited States for the Photosynthesis Process. Bulletin of the Chemical Society of Japan, 2020, 93, 1509-1519.	2.0	8
11995	Generalized Charge Decomposition Analysis (GCDA) Method. Journal of Advances in Physical Chemistry, 2015, 04, 111-124.	0.1	134
11996	Structure of Free Radical in ³ -Irradiated 21-Hydroxyprogesterone (Deoxycorticosterone) Single Crystals. ESR/ENDOR and DFT Studies. Acta Physica Polonica A, 2005, 108, 119-126.	0.2	6
11997	An Integrated Computational Approach to Rationalize the Activity of Non-Zinc-Binding MMP-2 Inhibitors. PLoS ONE, 2012, 7, e47774.	1.1	7
11998	Unique Kinase Catalytic Mechanism of AceK with a Single Magnesium Ion. PLoS ONE, 2013, 8, e72048.	1.1	7
11999	Synthesis, Spectral Characterization and Crystals Structure of some Arsane Derivatives of Gold (I) Complexes: A Comparative Density Functional Theory Study. PLoS ONE, 2015, 10, e0119620.	1.1	4
12000	Flavonoids in Microheterogeneous Media, Relationship between Their Relative Location and Their Reactivity towards Singlet Oxygen. PLoS ONE, 2015, 10, e0129749.	1.1	14
12001	In Vitro Protective Effect and Antioxidant Mechanism of Resveratrol Induced by Dapsone Hydroxylamine in Human Cells. PLoS ONE, 2015, 10, e0134768.	1.1	39
12002	SiO Desorption Kinetics of Si(111) Surface Oxidation Studied by Real-Time Photoelectron Spectroscopy. E-Journal of Surface Science and Nanotechnology, 2013, 11, 116-121.	0.1	2
12003	Diazo-pyrazole analogues as photosensitizers in dye sensitised solar cells: tuning for a better photovoltaic efficiency using a new modelling strategy using experimental and computational data. Zeitschrift Fur Physikalische Chemie, 2021, 235, 1227-1245.	1.4	11
12005	Account of surface contribution to thermodynamic properties of lead selenide films. Semiconductor Physics, Quantum Electronics and Optoelectronics, 2019, 22, 156-164.	0.3	1
12006	ĐšĐ²Đ°Đ½Ñ,Đ¾Đ²Đ¾¾-Ñ...Ñ-Đ¼Ñ-Ñ‡Đ½Đµ ĐĐ¾ÑĐ»Ñ-ĐĐ¶ĐµĐ½Đ½Ñ•Đ¼ĐµÑ...Đ°Đ½Ñ-Đ.Đ¼Ñf Ñ€ĐµĐ°ĐÑ†Ñ-Ñ- N-Ñ†Đ		
12008	Chiral Peculiar Properties of Self-Organization of Diphenylalanine Peptide Nanotubes: Modeling Of Structure and Properties. Mathematical Biology and Bioinformatics, 2019, 14, 94-125.	0.1	11
12009	DFT Based Quantum Chemical Descriptors of 1-Substituted TH ¹ 2C, DH ¹ 2C, I ² C Derivatives. Cumhuriyet Science Journal, 2017, 38, 647-660.	0.1	8
12010	A Computational Study of 1-substituted methyl 9-methyl-9H-pyrido[3,4-b]indole-3-carboxylate: Quantum Chemical Descriptors, FMO and NBO Analysis. Cumhuriyet Science Journal, 0, , 138-155.	0.1	17
12011	DFT ile benzimidazol t ¹ 4revlerinin korozyon inhibit ¹ 4r ¹ 4 olarak incelenmesi. Cumhuriyet Science Journal, 2019, 40, 396-405.	0.1	15
12012	Baz ¹ Fenolik Bile ¹ Yüklerin Yo ¹ Yunluk Fonksiyonu Y ¹ ntemi ile Antioksidan Aktivitelerinin Tayin Edilmesi. Journal of Natural and Applied Sciences, 0, 23, 139-146.	0.1	1

#	ARTICLE	IF	CITATIONS
12034	Quantitative Structure Anti-Cancer Activity Relationship (QSAR) of a Series of Ruthenium Complex Azopyridine by the Density Functional Theory (DFT) Method. Computational Molecular Bioscience, 2017, 07, 19-31.	0.6	8
12035	Non Local Corrections to the Electronic Structure of Non Ideal Electron Gases: The Case of Graphene and Tyrosine. Journal of Modern Physics, 2013, 04, 522-527.	0.3	2
12036	Understanding the Relativistic Generalization of Density Functional Theory (DFT) and Completing It in Practice. Journal of Modern Physics, 2016, 07, 911-919.	0.3	9
12037	Theoretical Studies of Geometries of Hexafluoro-1,3-butadiene, Tetrafluoro-1,3-butadiene, and Difluoro-1,3-butadiene Compounds. Bulletin of the Korean Chemical Society, 2004, 25, 452-459.	1.0	6
12038	Experimental and Theoretical Investigations of Spectral, Tautomerism and Acid-Base Properties of Schiff Bases Derived from Some Amino Acids. Bulletin of the Korean Chemical Society, 2010, 31, 850-858.	1.0	12
12039	Influence of Exchange-Correlation Functional in the Calculations of Vertical Excitation Energies of Halogenated Copper Phthalocyanines using Time-Dependent Density Functional Theory (TD-DFT). Bulletin of the Korean Chemical Society, 2013, 34, 2276-2280.	1.0	9
12040	A Gas-Phase Investigation of Oxygen-Hydrogen Exchange Reaction of $O(^3P) + C_2H_5 \rightarrow H(^2S) + C_2H_4O$. Bulletin of the Korean Chemical Society, 2014, 35, 839-844.	1.0	4
12041	DFT Studies on Hydrogen Bonding in Water Complexes of Amino-substituted Pyridine. Journal of the Korean Chemical Society, 2003, 47, 96-103. Interaction of Proline with Cu^+ and Cu^{2+} Ions in the Gas Phase. Gab Yong Lee* Department of Life Chemistry, Catholic University of Daegu, Gyeongsan 712-702, Korea (Received March 3,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 437 Td	0.2	1
12042	biological processes of living systems, including oxidation, dioxygen transport, and charge transfer. The study of interactions between the metal ion and amino acids has attracted considerable attention from experimental and theoretical viewpoints. Journal of the Korean Chemical Society, 2009, 53, 257-	0.2	4
12043	Theoretical Studies of Hydrogen Bond Interactions in 4-Substituted Benzoic Acids Dimers. Journal of the Korean Chemical Society, 2011, 55, 392-399.	0.2	2
12044	A DFT Study of the Intramolecular Hydrogen Bonding of Alanine and Its Effects on Ionization Energies. Journal of the Korean Chemical Society, 2015, 59, 541-544.	0.2	1
12045	Mechanisms of Mutagenic DNA Nucleobase Damages and Their Chemical and Enzymatic Repairs Investigated by Quantum Chemical Methods. , 0, , .		1
12046	Microscopic interactions between ivermectin and key human and viral proteins involved in SARS-CoV-2 infection. Physical Chemistry Chemical Physics, 2021, 23, 22957-22971.	1.3	11
12047	PEG-400 mediated synthesis, computational, antibacterial and antifungal studies of fluorinated pyrazolines. Current Research in Green and Sustainable Chemistry, 2021, 4, 100172.	2.9	12
12048	Color tuning of di-boron derived TADF emitters: molecular design and property prediction. Journal of Materials Chemistry C, 2021, 9, 15309-15320.	2.7	10
12049	The aqueous interaction of neodymium with two omnixistent biomoieties – a mechanistic understanding by experimental and theoretical studies. Dalton Transactions, 2021, 50, 16191-16204.	1.6	3
12050	QM/MM modeling of class A β -lactamases reveals distinct acylation pathways for ampicillin and cefalexin. Organic and Biomolecular Chemistry, 2021, 19, 9182-9189.	1.5	7
12051	Attaining record-high magnetic exchange, magnetic anisotropy and blocking barriers in dilanthanofullerenes. Chemical Science, 2021, 12, 14207-14216.	3.7	16

#	ARTICLE	IF	CITATIONS
12052	Modelling of the Electronic and Vibrational Structure. Springer Theses, 2021, , 37-63.	0.0	0
12053	Excitation wavelength-dependent room-temperature phosphorescence: unusual properties of novel phosphinoamines. <i>Molecular Systems Design and Engineering</i> , 2021, 6, 1056-1065.	1.7	15
12054	Theoretical Study of Magnetic Phase Transition In $\text{La}_2/3\text{Mn}_1/3\text{MnO}_3$ (M=Ca, Sr) Membranes Through Strain and Doping. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12055	Characterization of Light-Induced, Short-Lived Interacting Radicals in the Active Site of Flavoprotein Ferredoxin-NADP ⁺ Oxidoreductase. <i>Journal of the American Chemical Society</i> , 2021, 143, 2757-2768.	6.6	12
12056	Solvent effect on the Molecular structure and Global, Local and Dual Descriptors: A Density Functional Theory Study. <i>Asian Journal of Research in Chemistry</i> , 2021, , 305-315.	0.2	0
12057	First-principles study of Ti-doped sapphire. I. Formation and optical transition properties of titanium pairs. <i>Physical Review B</i> , 2021, 104, .	1.1	8
12058	Synthesis, Spectral Characterization, Electronic Structure and Biological Activity Screening of the Schiff Base 4-((4-Hydroxy-3-Methoxy-5-Nitrobenzylidene)Amino)-N-(Pyrimidin-2-yl)Benzene Sulfonamide from 5-Nitrovaniline and Sulphadiazene. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-18.	1.4	26
12059	Theoretical Investigation of the Effect of Alkylation and Bromination on Intersystem Crossing in BODIPY-Based Photosensitizers. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11617-11627.	1.2	8
12060	Local hybrid functionals augmented by a strong-correlation model. <i>Journal of Chemical Physics</i> , 2021, 155, 144101.	1.2	12
12061	Preferential solvation and optical properties of eumelanin building blocks in binary mixture of methanol and water. <i>Journal of Chemical Physics</i> , 2021, 155, 174504.	1.2	3
12062	First-Principles Simulation Study on the Weakening of Silane Coupling to Silica under Alkaline Conditions. <i>Journal of Physical Chemistry C</i> , 2021, 125, 22907-22916.	1.5	4
12063	Electropolymers of 4-(thieno[3,2-b]thiophen-3-yl)benzotrile extended with thiophene, 3-hexylthiophene and EDOT moieties; their electrochromic applications. <i>Polymer</i> , 2021, 235, 124286.	1.8	6
12064	Facile synthesis of some 5-(3-substituted-thiophene)-pyrimidine derivatives and their pharmacological and computational studies. <i>Chimica Techno Acta</i> , 2021, 8, .	0.3	4
12065	Metal-free catalysis for the reaction of nitrogen dioxide dimer with phenol: An unexpected favorable source of nitrate and aerosol precursors in vehicle exhaust. <i>Chemosphere</i> , 2021, , 132705.	4.2	3
12066	Acceleration Mechanisms of C-H Bond Functionalization Catalyzed by Electron-Deficient CpRh(III) Complexes. <i>ACS Catalysis</i> , 2021, 11, 13591-13602.	5.5	21
12067	Role of a 3D Structure in Energy Transfer in Mixed-Ligand Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2021, 125, 22998-23010.	1.5	15
12068	Evolution of the electronic structure in open-shell donor-acceptor organic semiconductors. <i>Nature Communications</i> , 2021, 12, 5889.	5.8	47
12069	Nazarov Cyclizations Catalyzed by BINOL Phosphoric Acid Derivatives: Quantum Chemistry Struggles To Predict the Enantioselectivity. <i>Journal of Organic Chemistry</i> , 2022, 87, 1710-1722.	1.7	5

#	ARTICLE	IF	CITATIONS
12070	Gas-phase ion-molecule interactions in a collision reaction cell with triple quadrupole-inductively coupled plasma mass spectrometry: Investigations with N ₂ O as the reaction gas. <i>Spectrochimica Acta, Part B: Atomic Spectroscopy</i> , 2021, 186, 106309.	1.5	15
12071	Assessing Tetrel-Based Neutral Frustrated Lewis Pairs for Catalytic Hydrogenation. <i>Journal of Physical Chemistry C</i> , 2021, 125, 22522-22530.	1.5	4
12072	Structural, vibrational, electronic properties, hirshfeld surface analysis topological and molecular docking studies of N-[2-(diethylamino)ethyl]-2-methoxy-5-methylsulfonylbenzamide. <i>Heliyon</i> , 2021, 7, e08186.	1.4	14
12073	Theoretical investigation of emodin conjugated doped B ₁₂ N ₁₂ nanocage by means of DFT, QTAIM and PCM analysis. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 136, 115027.	1.3	36
12074	Synthesis of Cu(II) complexes by N,O-donor ligand transformation and their catalytic role in visible-light-driven alcohol oxidation. <i>Applied Organometallic Chemistry</i> , 2022, 36, e6450.	1.7	6
12075	Waste-to-Energy: Production of Fuel Gases from Plastic Wastes. <i>Polymers</i> , 2021, 13, 3672.	2.0	3
12076	Lowest Triplet and Singlet States in N-Methylacridone and N ² -Dimethylquinacridone: Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8777-8790.	1.1	2
12077	Exploring Dyson's Orbitals and Their Electron Binding Energies for Conceptualizing Excited States from Response Methodology. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9963-9972.	2.1	11
12078	Gas-Phase Fluorination of Hexagonal Boron Nitride. <i>Advanced Materials</i> , 2021, 33, e2106084.	11.1	10
12079	General Construction of Thioamides under Mild Conditions: A Stepwise Proton Transfer Process Mediated by EDTA. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 6015.	1.2	4
12080	Modeling Spectral Tuning in Red Fluorescent Proteins Using the Dipole Moment Variation upon Excitation. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5125-5132.	2.5	2
12081	Comparing Properties of Common Bioinorganic Ligands with Switchable Variants of Cytochrome c. <i>Inorganic Chemistry</i> , 2021, , .	1.9	2
12082	Synthesis of a Negative Photochrome with High Switching Quantum Yields and Capable of Singlet-Oxygen Production and Storage. <i>Chemistry - A European Journal</i> , 2021, 27, 16642-16653.	1.7	6
12083	Simulation and Computer Study of Structures and Physical Properties of Hydroxyapatite with Various Defects. <i>Nanomaterials</i> , 2021, 11, 2752.	1.9	23
12084	First-principles study of Ti-doped sapphire. II. Formation and reduction of complex defects. <i>Physical Review B</i> , 2021, 104, .	1.1	6
12085	Investigation of bis(perfluoro-tert-butoxy) halogenates(I/III). <i>Chemistry - A European Journal</i> , 2021, 27, 17676.	1.7	1
12086	Ruthenium (II) Complexes Bearing Heteroleptic Terpyridine Ligands: Syntheses, Photophysics and Solar Energy Conversion. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 5014.	1.0	9
12087	The Reaction N ₂ + CH ₃ CCH (Methylacetylene): A Combined Crossed Molecular Beams and Theoretical Investigation and Implications for the Atmosphere of Titan. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8846-8859.	1.1	12

#	ARTICLE	IF	CITATIONS
12088	Dirhenium(III,III) trithiocarbamate complexes: experimental and theoretical investigation. <i>Transition Metal Chemistry</i> , 2021, 46, 583-591.	0.7	3
12089	Effects of surface species and homogeneous reactions on rates and selectivity in ethane oxidation on oxide catalysts. <i>AIChE Journal</i> , 2021, 67, e17483.	1.8	5
12090	Molecular Survey of Strongly and Weakly Interfacially Active Asphaltenes: An Intermolecular Force Field Approach. <i>Energy & Fuels</i> , 2021, 35, 17424-17433.	2.5	5
12091	Nature of the Ligand-Centered Triplet State in Gd ³⁺ Diketonate Complexes as Revealed by Time-Resolved EPR Spectroscopy and DFT Calculations. <i>Inorganic Chemistry</i> , 2021, 60, 15141-15150.	1.9	4
12092	Photochemistry of Heteroleptic 1,4,5,8-Tetraazaphenanthrene- and Bi-1,2,3-triazolyl-Containing Ruthenium(II) Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 15768-15781.	1.9	9
12093	Identification of DNA Bases and Their Cations in Astrochemical Environments: Computational Spectroscopy of Thymine as a Test Case. <i>Frontiers in Astronomy and Space Sciences</i> , 2021, 8, .	1.1	0
12094	Photochemistry of Thymine in Protic Polar Nanomeric Droplets Using Electrostatic Embedding TD-DFT/MM. <i>Molecules</i> , 2021, 26, 6021.	1.7	1
12095	Theoretical evaluation of the hydrolysis of conventional nerve agents and novichok agents. <i>Chemical Physics Letters</i> , 2021, 785, 139116.	1.2	12
12096	Perspective on "The activated complex in chemical reactions", 2000, , 190-195.		1
12097	An experimental and theoretical approach to the study of the properties of parabanic acid and related compounds: synthesis and crystal structure of diethylimidazolidine-2-selone-4,5-dione. <i>Canadian Journal of Chemistry</i> , 2000, 78, 1147-1157.	0.6	13
12104	Density Functional Study for Chemical Reaction between Cr and Fe with Sodium Diethyldithiocarbamate (NaDDC). <i>Shinku/Journal of the Vacuum Society of Japan</i> , 2006, 49, 390-391.	0.2	1
12106	Development of the multi-component hybrid density functional theory. , 2006, , 1536-1539.		0
12107	Recent Trends in Quantum Chemical Calculations for Surface-Molecule Interacting Systems. <i>Hyomen Kagaku</i> , 2007, 28, 150-159.	0.0	0
12109	Catalytic Roles of V ₂ O ₅ on Benzene Ring Decomposition using Ab Initio Molecular Orbital Method. <i>Journal of Environmental Chemistry</i> , 2007, 17, 37-45.	0.1	0
12110	Density Functional Theory and Car-Parrinello Molecular Dynamics Methods. <i>Advances in Photosynthesis and Respiration</i> , 2008, , 487-499.	1.0	1
12111	Defects in CMOS Gate Dielectrics. , 2008, , .		0
12112	Density Functional Calculation of the Structure and Electronic Properties of Cu _n O _n (n=1-4) Clusters. <i>Lecture Notes in Computer Science</i> , 2009, , 122-130.	1.0	0
12113	Multi-Scale Modeling of CO Oxidation on Pt-Based Electrocatalysts. <i>Topics in Applied Physics</i> , 2009, , 533-549.	0.4	1

#	ARTICLE	IF	CITATIONS
12115	A Quasirelativistic Two-component Density Functional and Hartree-Fock Program. , 2010, , 123-136.		0
12116	Orbital-dependent Representation of Correlation Energy Functional. , 2010, , 165-176.		0
12117	Some Recent Studies on the Local Reactivity of O ₂ on Pt ₃ Nanoislands Supported on Mono- and Bi-Metallic Backgrounds. Modern Aspects of Electrochemistry, 2010, , 203-242.	0.2	0
12118	Density-Functional Theory with Orbital-Dependent Functionals: Exact-exchange Kohn-Sham and Density-Functional Response Methods. , 2010, , 35-52.		0
12120	Origin of Exo/Endo Selectivity in the Intramolecular Diels-Alder Reaction. Bulletin of the Korean Chemical Society, 2010, 31, 2527-2530.	1.0	0
12121	Some Practical Considerations for Density Functional Theory Studies of Chemistry at Metal Surfaces. , 2011, , .		4
12123	THE CRYSTAL STRUCTURE AND QUANTUM MECHANICAL TREATMENT OF THE ANTI-CANCER AGENT FLAVOPIRIDOL (HYDROCHLORIDE) AND THE CHROMONE ALKALOID ROHITUKINE. Proceedings of the Nova Scotian Institute of Science, 2011, 46, .	0.0	0
12124	Density Functional Study of the Origin of the Strongly Delocalized Electronic Structure of the CuA Site in Cytochrome c Oxidase. Progress in Theoretical Chemistry and Physics, 2012, , 513-524.	0.2	0
12125	Synthesis and Theoretical Study of Zinc(II) and Nickel(II)-Complexes of 5-Methoxyisatin 3-[N-(4-chlorophenyl)thiosemicarbazone]. ITB Journal of Science, 2012, 44, 35-50.	0.1	0
12126	Telluroformaldehyde and its derivatives: structures, ionization potentials, electron affinities and singlet-triplet gaps of the X ₂ CTe and XYCTe (X,Y = H, F, Cl, Br, I and CN) species. Highlights in Theoretical Chemistry, 2012, , 43-74.	0.0	0
12127	Discovery of Chemical Principles:Symmetry Rules for Degenerate Excitations. Journal of Computer Chemistry Japan, 2012, 11, 1-16.	0.0	4
12128	Ab initio classical trajectory calculations of 1,3-cyclobutanedione radical cation dissociation. Highlights in Theoretical Chemistry, 2013, , 5-9.	0.0	0
12129	Theoretical investigation of molecular excited states in polar organic monolayers via an efficient embedding approach. Highlights in Theoretical Chemistry, 2013, , 121-128.	0.0	0
12130	Thermal and environmental effects on Oligothiophene low-energy singlet electronic excitations in dilute solution: a theoretical and experimental study. Highlights in Theoretical Chemistry, 2013, , 185-198.	0.0	0
12131	Impact of DFT functionals on the predicted magnesium-DNA interaction: an ONIOM study. Highlights in Theoretical Chemistry, 2013, , 271-279.	0.0	0
12132	Effects of mutations on the absorption spectra of copper proteins: a QM/MM study. Highlights in Theoretical Chemistry, 2014, , 39-47.	0.0	0
12133	Quantum Chemical Studies of the Ground States of the Metal Centres in Haem-Copper Oxidases. Current Inorganic Chemistry, 2012, 2, 316-324.	0.2	0
12134	Theoretical Foundation. Springer Theses, 2013, , 17-62.	0.0	0

#	ARTICLE	IF	CITATIONS
12153	Density Functional Theory: Improving the Functionals, Extending the Applications. , 1996, , 359-394.		1
12154	Subhamiltonian Methods. , 1996, , 33-54.		1
12155	Correlation Energy in a High-Density Limit from Adiabatic Connection Perturbation Theory. , 1998, , 113-123.		0
12156	A theoretical model of the Si/SiO ₂ interface. , 1998, , 131-145.		1
12158	Non-local Exchange and Correlation. Springer Series in Solid-state Sciences, 2015, , 163-195.	0.3	0
12159	The Quantum Chemical Calculations of Some Thiazole Derivatives. , 0, , .		2
12160	A Material Design on Radioactive Cesium Adsorbent: Cs _{1-x} Na _x Mn ^{II} (CN) ₃ Prussian Blue Analogue. Journal of Computer Chemistry Japan, 2015, 14, 36-42.	0.0	0
12162	First-Principles Simulations of Bulk Crystal and Nanolayer Properties. Nanoscience and Technology, 2015, , 113-214.	1.5	0
12164	Dielectric Spectroscopic Studies of Propylene Glycol/Aniline Mixtures at Temperatures Between 303K to 323K. International Journal of Engineering Research & Technology, 2015, V4, .	0.2	1
12165	Theoretical Insights Elucidate Novel Active Phosphonate Estersâ€”Cephalosporin Antibioticsâ€™ Intermediate. Open Journal of Inorganic Chemistry, 2016, 06, 219-228.	0.7	0
12166	Nanocluster-Assembled Materials. , 2016, , 127-162.		0
12167	ADSORPTION OF RARE GAS ATOMS ON Cu (111) SURFACE. International Journal of Innovations in Biological and Chemical Science, 0, 8, 1-12.	0.0	0
12168	Electronic and carrier transport properties of small molecule donors. Multiscale and Multiphysics Mechanics, 2016, 1, 305-326.	0.3	0
12169	Symulacje ab-initio warstwy grafenowej wykorzystywanej w detektorze IR. Elektronika, 2016, 1, 33-34.	0.0	0
12170	Mechanistic Studies on Pd(OAc) ₂ -C ₆₀ catalyzed Meta-C-H Activation Reaction. Springer Theses, 2017, , 43-62.	0.0	0
12171	Mechanistic Studies on Pd(MPAA)-Catalyzed Meta- and Ortho-C-H Activation Reactions. Springer Theses, 2017, , 63-81.	0.0	0
12172	Electronic and carrier transport properties of small molecule donors. Coupled Systems Mechanics, 2017, 6, 75-96.	0.4	0
12174	Synthesis, Characterisation and DFT Calculations of Azo-Imine Dyes. Journal of the Turkish Chemical Society, Section A: Chemistry, 0, , 159-178.	0.4	3

#	ARTICLE	IF	CITATIONS
12175	Conformation of Gemcitabine: An Experimental NMR and Theoretical DFT Study. <i>Scientia Iranica</i> , 2017, .	0.3	0
12176	<i>Molecular Wires</i> . Springer Theses, 2018, , 65-82.	0.0	0
12177	Efecto de la estructura molecular sobre el espectro electrónico vertical de la oxoglaucina. <i>Revista Colombiana De Quimica</i> , 2018, 47, 64-76.	0.2	0
12178	Molecular Structure, Electronic Structure, Properties and Analyses of Five Azopyridine Ruthenium Complexes $\hat{\Gamma}^{\pm}$ -Cl, $\hat{\Gamma}^2$ -Cl, $\hat{\Gamma}^3$ -Cl, $\hat{\Gamma}^{\prime}$ -Cl and $\hat{\Gamma}^{\mu}$ -Cl of RuCl ₂ (4,6-Dimethyl-Phenylazopyridine) ₂ as Potential Cancer Drugs: DFT and TD-DFT Investigations. <i>Computational Chemistry</i> , 2018, 06, 27-46.	0.2	0
12179	Theoretical investigation of carbon dioxide capture by aqueous boric acid solution: A termolecular reaction mechanism. <i>Journal of Boron</i> , 0, , .	0.0	0
12181	Theoretical Investigation of Structural and Electronic Properties of Ruthenium Azopyridine Complexes Dyes for Photovoltaic Applications by Using DFT and TD-DFT Methods. <i>European Scientific Journal</i> , 2018, 14, 424.	0.0	2
12182	4-Klorometil-6,8-dimetilkumarin Bileşiminin Sentezi ve Teorik Kimyasal Hesaplamalar. <i>Bitlis Eren Üniversitesi Fen Bilimleri Dergisi</i> , 2018, 7, 311-319.	0.1	3
12183	Nitridation-Etch of Silicon Oxide in Fluorocarbon/Nitrogen Plasma: A Computational Study. <i>Journal of Microelectronic Manufacturing</i> , 2019, 2, 1-8.	0.2	0
12184	Effect of the position of an epoxy group on the H-graphene cluster properties: The density functional theory calculations. <i>Journal of Physical Studies</i> , 2019, 23, .	0.2	0
12185	Impact of Nicotine Consumption on Hyper Acidic Patients Taking PPI: An <i>In-Vitro</i> and Computational Analysis. <i>Health</i> , 2019, 11, 129-141.	0.1	2
12189	Spin Crossover in Iron(II) Complexes with Mixed Nitrogen-Sulfur Coordination: DFT Modeling. <i>IFMBE Proceedings</i> , 2020, , 33-36.	0.2	0
12190	First principle investigation of pristine and TM adsorbed B6 nanocluster: A comparative DFT study. , 2019, , .		0
12192	Binding Energies of N-Bearing Astrochemically-Relevant Molecules on Water Interstellar Ice Models. A Computational Study. <i>Lecture Notes in Computer Science</i> , 2020, , 683-692.	1.0	2
12193	Predicting band gaps of semiconductors with quantum chemistry. <i>EPJ Web of Conferences</i> , 2020, 246, 00006.	0.1	0
12194	Environmentally Friendly Syntheses of Imines Applying the Pressure Reduction Technique: Reaction Cases of Less Reactive Amines and Studies by Computational Chemistry. <i>Green and Sustainable Chemistry</i> , 2020, 10, 1-17.	0.8	0
12195	Neutral Lipophilic Palladium(II) Complexes and their Applications in Electrocatalytic Hydrogen Production and C-C Coupling Reactions. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 813-822.	1.0	1
12196	Biomolecular Simulation: A Perspective from High Performance Computing. <i>Israel Journal of Chemistry</i> , 2020, 60, 694-704.	1.0	2
12197	Nuclear quantum and H/D isotope effects on three-centered bonding diborane: Path integral molecular dynamics simulations. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26179.	1.0	1

#	ARTICLE	IF	CITATIONS
12199	Physical origin of the one-quarter exact exchange in density functional theory. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 385501.	0.7	2
12200	Electronic structural properties of amino/hydroxyl functionalized imidazolium-based bromide ionic liquids. <i>Open Chemistry</i> , 2020, 18, 576-583.	1.0	2
12201	Electrophilic Aromatic Synthesis of Radioiodinated Aripiprazole: Experimental and DFT Investigations. <i>Current Organic Synthesis</i> , 2020, 17, 295-303.	0.7	1
12202	Removal of nafcillin sodium monohydrate from aqueous solution by hydrogels containing nanocellulose: An experimental and theoretical study. <i>Journal of Molecular Liquids</i> , 2022, 347, 117946.	2.3	5
12203	Beyond Conformational Control: Effects of Noncovalent Interactions on Molecular Electronic Properties of Conjugated Polymers. <i>Jacs Au</i> , 2021, 1, 2182-2187.	3.6	8
12204	Combination of docetaxel and newly synthesized 9-Br-trimethoxybenzyl-noscapine improve tubulin binding and enhances antitumor activity in breast cancer cells. <i>Computers in Biology and Medicine</i> , 2021, 139, 104996.	3.9	2
12205	Mono- and dinuclear zinc complexes bearing identical bis(thiosemicarbazone) ligand that exhibit alkaline phosphatase-like catalytic reactivity. <i>Journal of Biological Inorganic Chemistry</i> , 2021, , 1.	1.1	1
12206	Second-Order CASSCF Algorithm with the Cholesky Decomposition of the Two-Electron Integrals. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6819-6831.	2.3	12
12207	DFT quest for mechanism and stereoselectivity in B(C ₆ F ₅) ₃ -catalyzed cyclopropanation of alkenes with aryldiazoacetates. <i>Molecular Catalysis</i> , 2021, 516, 111980.	1.0	3
12208	Bottom-up dust nucleation theory in oxygen-rich evolved stars. <i>Astronomy and Astrophysics</i> , 2022, 658, A167.	2.1	22
12209	Electronic second hyperpolarizability of alkaline earth metal chains end capped with $\hat{\alpha}^{\text{NH}_2}$ and $\hat{\alpha}^{\text{CN}}$. <i>Journal of the Indian Chemical Society</i> , 2021, 98, 100234.	1.3	2
12210	Temperature and Time-resolved XANES Studies of Novel Valence Tautomeric Cobalt Complex. <i>Chemistry Letters</i> , 2021, 50, 1933-1937.	0.7	7
12211	Unveiling the Electronic Structure of Grain Boundaries in Anatase with Electron Microscopy and First-Principles Modeling. <i>Nano Letters</i> , 2021, 21, 9217-9223.	4.5	8
12212	Microhydration of sorbitan monostearate (Span 60) investigated using hybrid QM/MM calculations in the gas phase. <i>Surface Science</i> , 2022, 716, 121977.	0.8	1
12213	Mechanistic insight into the isomerization of allyl alcohol catalyzed by the Co(II)-PNP catalyst: Crucial role of spectator ligand. <i>Molecular Catalysis</i> , 2021, 516, 111957.	1.0	0
12214	Atomistic Modeling of Oxide Defects. , 2020, , 609-648.		4
12215	First-Principles Simulations of Bulk Crystal and Nanolayer Properties. <i>Nanoscience and Technology</i> , 2020, , 123-219.	1.5	0
12216	A diagonalization-free optimization algorithm for solving $\langle \text{sc} \rangle \text{Kohn-Sham} \langle / \text{sc} \rangle$ equations of $\langle \text{sc} \rangle \text{closed-shell} \langle / \text{sc} \rangle$ molecules. <i>Journal of Computational Chemistry</i> , 2021, 42, 492-504.	1.5	0

#	ARTICLE	IF	CITATIONS
12217	Theoretical and structural studies of a stable dinuclear sodium complex of dicoumarol - 3,3- λ^2 -(pyridin-3-ylmethanediyl)bis(4-hydroxy-2H-chromen-2-one). Journal of Molecular Structure, 2020, 1222, 128956.	1.8	0
12218	IRMPD spectroscopy and quantum chemistry calculations on mono- and bi-metallic complexes of acetylacetonate ligands with aluminum, iron, and ruthenium ions. Journal of Chemical Physics, 2020, 153, 234303.	1.2	4
12219	Heteroleptic dmit nickel complexes with bis(diphenylphosphanyl)amine ligands as robust molecular electrocatalysts for hydrogen evolution. Applied Organometallic Chemistry, 2021, 35, .	1.7	3
12220	Thermochemistry of neutral and anionic sulfur fluorides SF _n (n = 1-6): Revisited with theoretical G4/W1/W2 composite methods and the roles of metastable conformer of SF ₄ ⁻ anion. AIP Advances, 2020, 10, 125112.	0.6	2
12221	Unraveling Structural and Optical Properties of Two-Dimensional Mo ₂ W ₂ S ₂ Alloys. Journal of Physical Chemistry C, 2021, 125, 774-781.	1.5	17
12222	On the Mechanism of Bioinspired Formation of Inorganic Oxides: Structural Evidence of the Electrostatic Nature of the Interaction between a Mononuclear Inorganic Precursor and Lysozyme. Biomolecules, 2021, 11, 43.	1.8	4
12223	Femtosecond intersystem crossing to the reactive triplet state of the 2,6-dithiopurine skin cancer photosensitizer. Physical Chemistry Chemical Physics, 2021, 23, 25048-25055.	1.3	3
12224	A bis indole analog molecule fluorescent probe for living cell staining. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 424, 113613.	2.0	5
12225	Synthesis of a versatile Schiff base 4-((2-hydroxy-3,5-diiodobenzylidene)amino) benzenesulfonamide from 3,5-diiodosalicylaldehyde and sulfanilamide, structure, electronic properties, biological activity prediction and experimental antimicrobial properties. Journal of Molecular Structure, 2022, 1250, 131700.	1.8	18
12226	Energetic Ground State Calculations, Electronic Band Structure at Surfaces. Springer Handbooks, 2020, , 471-498.	0.3	0
12227	Carbazol-phenyl-phenothiazine-based sensitizers for dye-sensitized solar cells. Journal of Materials Chemistry A, 2021, 9, 26311-26322.	5.2	6
12228	The porphyrin center as a regulator for metal-ligand covalency and π hybridization in the entire molecule. Physical Chemistry Chemical Physics, 2021, 23, 24765-24772.	1.3	11
12229	Aminopolycarboxylates in trivalent f-element separations. Fundamental Theories of Physics, 2021, 60, 1-162.	0.1	2
12230	Schiff Bases and their Copper(II) Complexes Derived from Cinnamaldehyde and Different Hydrazides: Synthesis and Antibacterial Properties. Journal of Transition Metal Complexes, 2020, 3, 1-9.	0.5	3
12231	A Theoretical Investigation of the Reaction Between Glycolaldehyde and H ⁺ and Implications for the Organic Chemistry of Star Forming Regions. Lecture Notes in Computer Science, 2020, , 730-743.	1.0	0
12232	Structural, optical and magnetic properties of B ₈ , FeB ₈ , CoB ₈ , NiB ₈ nanoclusters: A DFT study. , 2020, , .		0
12234	Anomaly in the stability of the hydroxides of icosagens (B and Al) and their noble gas (Xe and Rn) derivatives: a comparative study. Physical Chemistry Chemical Physics, 2020, 22, 14109-14124.	1.3	6
12235	Review Article on Density Functional Theory. Springer Proceedings in Physics, 2020, , 211-220.	0.1	6

#	ARTICLE	IF	CITATIONS
12236	Singlet fission relevant energetics from optimally tuned range-separated hybrids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27060-27076.	1.3	7
12237	Establishing the accuracy of density functional approaches for the description of noncovalent interactions in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25558-25564.	1.3	5
12238	Photophysics of Faecal Pigments Stercobilin and Urobilin in Aliphatic Alcohols: Introduction of a Sensitive Method for their Detection using Solvent Phase Extraction and Fluorometry. <i>Analytical Methods</i> , 2021, 13, 5573-5588.	1.3	1
12239	Protein confinement fine-tunes the aggregation-induced emission in the human serum albumin. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26263-26272.	1.3	5
12240	Hungry for charge – how a beryllium scorpionate complex –eats– a weakly coordinating anion. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2020, 75, 503-508.	0.3	2
12241	Electronic and photoelectronic properties of N-(5-indazolyl)-arylsulfonamides molecules: DFT / TD-DFT study. , 2020, , .		2
12242	DFT and TD-DFT studies for optoelectronic properties of coumarin based donor–acceptor (D–A) dyes: applications in dye-sensitized solar cells (DSSCs). <i>Heliyon</i> , 2021, 7, e08339.	1.4	22
12243	Covalency of Trivalent Actinide Ions with Different Donor Ligands: Do Density Functional and Multiconfigurational Wavefunction Calculations Corroborate the Observed –Breaks–?. <i>Inorganic Chemistry</i> , 2021, 60, 17744-17757.	1.9	13
12244	Rh Complexes with Pincer Carbene CNC Lutidine-Based Ligands: Reactivity Studies toward H ₂ Addition. <i>Organometallics</i> , 0, , .	1.1	7
12245	Five-Fold Symmetric Pentaindolo– and Pentakis(benzoindolo)Corannulenes: Unique Structural Dynamics Derived from the Combination of Helical and Bowl Inversions. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	5
12246	Density Functional Theory Half-Electron Self-Energy Correction for Fast and Accurate Nonadiabatic Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 10886-10892.	2.1	10
12247	Prediction of reaction mechanism for OH radical-mediated phenol oxidation using quantum chemical calculation. <i>Chemosphere</i> , 2022, 291, 132763.	4.2	15
12248	Five-Fold Symmetric Pentaindolo– and Pentakis(benzoindolo)Corannulenes: Unique Structural Dynamics Derived from the Combination of Helical and Bowl Inversions. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	15
12249	Stability, optical and charge transport properties of saddle-shaped cyclooctatetrathiophene (COTh) isomers: a theoretical study. <i>Journal of Sulfur Chemistry</i> , 2022, 43, 180-192.	1.0	3
12250	A Localized Planarization Strategy in Hole Mobility Modulation of Disordered Triphenylamine–Based Organic Semiconductors. <i>Advanced Theory and Simulations</i> , 2021, 4, 2100236.	1.3	0
12251	Understanding Hygroscopicity of Theophylline via a Novel Cocrystal Polymorph: A Charge Density Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9736-9756.	1.1	6
12252	Theoretical Study of Circular Dichroism Spectra in the Vacuum-Ultraviolet. , 1999, , 93-119.		1
12253	Computational Studies of Mineral-Water Interfaces. , 0, , 26-100.		0

#	ARTICLE	IF	CITATIONS
12254	Effects of Hydrogen Passivation on Fullerene-Derived Si ₃₀ C ₃₀ Clusters. <i>Frontiers in Materials</i> , 2020, 7, .	1.2	0
12255	Determination of Pairwise Interaction of Atoms from the Interaction of an Adatom with Graphene. <i>Russian Journal of Inorganic Chemistry</i> , 2020, 65, 1373-1377.	0.3	1
12256	Benzoat esteri iÅŒeren kumarin yapÄ±lÄ± bileÅŒiÅŒin deneysel ve kuantum kimyasal hesaplamalarÄ±. <i>Bitlis Eren Åœeniversitesi Fen Bilimleri Dergisi</i> , 2020, 9, 1587-1595.	0.1	0
12257	Die grÄŒenbeschleunigte kinetische Racematspaltung sekundÄrer Alkohole. <i>Angewandte Chemie</i> , 2021, 133, 786-791.	1.6	4
12258	Position isomers of Ru(II) polypyridine complexes with tunable photophysical properties, aggregation-induced phosphorescence enhancement and application in triplet-triplet annihilated upconversion. <i>Dyes and Pigments</i> , 2020, 180, 108489.	2.0	4
12259	Structural and electronic properties of 3-[2-(3, 4-dimethoxy) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 547 Td (phenyl)-ethyl]-2-met (quantum chemical calculations) approach. <i>Molecular Crystals and Liquid Crystals</i> , 2020, 708, 98-120.	0.4	2
12260	Neutral nickel(II) complex bearing hemilabile N,S-donor ligands â€“ structural, Hirshfeld surfaces and DFT studies. <i>Molecular Crystals and Liquid Crystals</i> , 2020, 709, 98-110.	0.4	5
12261	Mechanism, reactivity, and selectivity in a palladium-catalyzed organosilicon-based cross coupling reaction. <i>Catalysis Science and Technology</i> , 2022, 12, 135-143.	2.1	3
12262	<i>O</i>-Acetylated sugars in the gas phase: stability, migration, positional isomers and conformation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1016-1022.	1.3	4
12263	Understanding gas absorption in multivalent ionic liquids via solute-solvent interaction analyses. <i>Chemical Physics Letters</i> , 2022, 786, 139204.	1.2	7
12264	Prominence of Cu in a plasmonic Cuâ€“Ag alloy decorated SiO ₂ @S-doped C ₃ N ₄ coreâ€“shell nanostructured photocatalyst towards enhanced visible light activity. <i>Nanoscale Advances</i> , 0, , .	2.2	8
12265	Can time-dependent double hybrid density functionals accurately predict electronic excitation energies of BODIPY compounds?. <i>Computational and Theoretical Chemistry</i> , 2022, 1207, 113531.	1.1	9
12266	Symmetry-Breaking Charge Separation in Phenylene-Bridged Perylenediimide Dimers. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7633-7643.	1.1	23
12267	KSSOLV-GPU: An efficient GPU-enabled MATLAB toolbox for solving the Kohn-Sham equations within density functional theory in plane-wave basis set. <i>Chinese Journal of Chemical Physics</i> , 2021, 34, 552-564.	0.6	9
12268	Benchmarking isotropic hyperfine coupling constants using (QTP) DFT functionals and coupled cluster theory. <i>Journal of Chemical Physics</i> , 2022, 156, 094107.	1.2	5
12269	Antioxidant activities of <i>Alyssum virgatum</i> plant and its main components. <i>Structural Chemistry</i> , 2022, 33, 267-279.	1.0	3
12270	Pd(II)-Catalyzed Synthesis of Benzocyclobutenes by Î ² -Methylene-Selective C(sp ³)â€“H Arylation with a Transient Directing Group. <i>Journal of the American Chemical Society</i> , 2021, 143, 20035-20041.	6.6	37
12271	Complexation of Np(V) with the Dicarboxylates, Malonate, and Succinate: Complex Stoichiometry, Thermodynamic Data, and Structural Information. <i>Inorganic Chemistry</i> , 2021, , .	1.9	1

#	ARTICLE	IF	CITATIONS
12272	Exploring DFT+U parameter space with a Bayesian calibration assisted by Markov chain Monte Carlo sampling. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	8
12273	Regioselective Stepwise Bromination of [14]Triphyrins(2.1.1) and Their Effects on Structural, Spectral, and Redox Properties. <i>Journal of Organic Chemistry</i> , 2021, 86, 17640-17650.	1.7	5
12274	Theoretical insights into the degradation of swep by hydroxyl radicals in atmosphere and water environment: Mechanisms, kinetics and toxicity. <i>Science of the Total Environment</i> , 2022, 816, 151651.	3.9	3
12275	BSE49, a diverse, high-quality benchmark dataset of separation energies of chemical bonds. <i>Scientific Data</i> , 2021, 8, 300.	2.4	9
12276	Two novel mono-hydroxyl pyranoanthocyanidins bearing dimethylamino substituent(s) for dye-sensitized solar cell. <i>Journal of Molecular Structure</i> , 2021, 1252, 132055.	1.8	7
12277	An inexpensive density functional theory based protocol to predict accurate ^{19}F NMR chemical shifts. <i>Journal of Computational Chemistry</i> , 2022, 43, 170-183.	1.5	5
12278	Generalised Kohn-Sham equations with accurate total energy and single-particle eigenvalue spectrum. <i>Journal of Chemical Physics</i> , 2021, 155, 224105.	1.2	3
12279	Synthesis and Structural Properties of NIR Absorbing Pyridine Containing Heptaphyrins. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	3
12280	On the Unexpected Accuracy of the M06L Functional in the Calculation of ^{13}C Spin Spin Coupling Constants. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7712-7723.	2.3	10
12281	Switching Effects in Metalloporphyrin System Due to the Withdrawal of Spin Symmetry. <i>Studies in Autonomic, Data-driven and Industrial Computing</i> , 2022, , 343-351.	0.4	0
12282	Optical Spectra of Oligofurans: A Theoretical Approach to the Transition Energies, Reorganization Energies, and the Vibronic Activity. <i>Molecules</i> , 2021, 26, 7163.	1.7	0
12283	Phenothiazine-based dyes containing imidazole with π -linkers of benzene, furan and thiophene: Synthesis, photophysical, electrochemical and computational investigation. <i>Journal of Molecular Structure</i> , 2022, 1251, 131959.	1.8	19
12284	A review of quantum chemical methods for treating energetic molecules. <i>Energetic Materials Frontiers</i> , 2021, 2, 292-305.	1.3	21
12285	Disproportionation of the Uranyl(V) Coordination Complexes in Aqueous Solution through Outer-Sphere Electron Transfer. <i>Inorganic Chemistry</i> , 2021, 60, 18832-18842.	1.9	4
12286	Synthesis, Characterization, Antioxidant and DFT Studies of Some Novel Schiff Base Compounds. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 47-63.	1.0	0
12287	Synthesis of Stable Nonaromatic Fluorenonephyrin Macrocyclic. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 3421-3427.	1.3	5
12288	Nitrite-enhanced N-nitrosamines formation during the simulated tetracycline polluted groundwater chlorination: Experimental and theoretical investigation. <i>Chemical Engineering Journal</i> , 2022, 431, 133363.	6.6	3
12289	Design, synthesis, and computational explorations of novel β -thiohydantoin nucleosides with cytotoxic activities. <i>Journal of Heterocyclic Chemistry</i> , 2022, 59, 664-685.	1.4	7

#	ARTICLE	IF	CITATIONS
12290	Extended Benchmark Set of Main-Group Nuclear Shielding Constants and NMR Chemical Shifts and Its Use to Evaluate Modern DFT Methods. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7602-7621.	2.3	37
12291	Linear Carbene Pyridine Copper Complexes with Sterically Demanding λ^2 -Bis(trityl)imidazolyliene: Syntheses, Molecular Structures, and Photophysical Properties. <i>Inorganic Chemistry</i> , 2021, 60, 18529-18543.	1.9	24
12292	Polaron in TiO ₂ from First Principles: A Review. <i>Advanced Theory and Simulations</i> , 2022, 5, 2100244.	1.3	10
12293	Assessing and rationalizing the performance of Hessian update schemes for reaction path Hamiltonian rate calculations. <i>Journal of Chemical Physics</i> , 2021, 155, 204112.	1.2	1
12294	DFT calculation, molecular docking, and molecular dynamics simulation study on substituted phenylacetamide and benzohydrazide derivatives. <i>Journal of Molecular Modeling</i> , 2021, 27, 359.	0.8	4
12295	Quantum chemical study of reaction mechanism between plutonium and nitrogen. <i>Journal of Molecular Modeling</i> , 2021, 27, 363.	0.8	1
12296	X-ray absorption spectroscopy of trivalent Eu, Gd, Tb, and Dy chlorides and oxchlorides. <i>Journal of Alloys and Compounds</i> , 2022, 897, 162629.	2.8	4
12297	Application of TD-DFT Theory to Studying Porphyrinoid-Based Photosensitizers for Photodynamic Therapy: A Review. <i>Molecules</i> , 2021, 26, 7176.	1.7	6
12298	Synthesis, in vitro and in silico antitumor evaluation of 3-(2,6-dichlorophenyl)-1,5-diphenylpentane-1,5-dione: Structure, spectroscopic, RDC, Hirshfeld and DFT based analyses. <i>Journal of Molecular Structure</i> , 2022, 1251, 132002.	1.8	8
12299	Glass-forming Schiff bases: Peculiar self-organizing systems with bifurcated hydrogen bonds. <i>Journal of Molecular Liquids</i> , 2021, , 118052.	2.3	2
12300	Elucidating the Glucokinase Activating Potentials of Naturally Occurring Prenylated Flavonoids: An Explicit Computational Approach. <i>Molecules</i> , 2021, 26, 7211.	1.7	17
12301	Hydrogen-bonded supramolecular assemblies of folic acid with simple hexoses. <i>Journal of Molecular Structure</i> , 2022, 1250, 131904.	1.8	0
12302	Triphenylamine/4,4'-Dimethoxytriphenylamine-Functionalized Thieno[3,2- <i>b</i>]thiophene Fluorophores with a High Quantum Efficiency: Synthesis and Photophysical Properties. <i>Journal of Physical Chemistry B</i> , 2021, 125, 13309-13319.	1.2	16
12303	Correlation Effects in Trimeric Acylphloroglucinols. <i>Computation</i> , 2021, 9, 121.	1.0	5
12304	The GW/BSE Method in Magnetic Fields. <i>Frontiers in Chemistry</i> , 2021, 9, 746162.	1.8	14
12305	Platinum Iodide-Catalyzed Formal Three-Component Cascade Cycloaddition Reactions between β^3 -Aminoalkynes and Electron-Deficient Alkynes. <i>Journal of Organic Chemistry</i> , 2021, 86, 16614-16624.	1.7	2
12306	Mechanisms and kinetics of citrate-promoted dissolution of a uranyl phosphate mineral. <i>Geochimica Et Cosmochimica Acta</i> , 2022, 318, 247-262.	1.6	3
12307	Graphene oxide-mediated the reduction of U(VI), Re(VII), Se(VI) and Se(IV) by Fe(II) in aqueous solutions investigated via combined batch, DFT calculation and spectroscopic approaches. <i>Chemical Engineering Journal</i> , 2022, 433, 133844.	6.6	19

#	ARTICLE	IF	CITATIONS
12308	Competitive nuclear quantum effect and H/D isotope effect on torsional motion of H ₂ O ₂ : An ab initio path integral molecular dynamics study. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113542.	1.1	2
12309	Calculating Entropies of Large Molecules in Aqueous Phase. <i>Journal of Chemical Theory and Computation</i> , 2021, , .	2.3	6
12310	Novel Third-Order Nonlinear Optical Materials with Craig-MÃ¶bius Aromaticity. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 11784-11789.	2.1	13
12311	Ligand-controlled divergent dehydrogenative reactions of carboxylic acids via C-H activation. <i>Science</i> , 2021, 374, 1281-1285.	6.0	64
12312	Glycerol-derived Solvents Containing Two or Three Distinct Functional Groups Enabled by Trifluoroethyl Glycidyl Ether. <i>AIChE Journal</i> , 0, , e17533.	1.8	8
12313	Resolving competing conical intersection pathways: time-resolved X-ray absorption spectroscopy of <i>cis</i> -1,3-butadiene. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1345-1354.	1.3	5
12314	Halide Perovskites for Photonics: Recent History and Perspectives. , 2021, , 1-28.		1
12315	A theoretical study of allopurinol drug sensing by carbon and boron nitride nanostructures: DFT, QTAIM, RDG, NBO and PCM insights. <i>RSC Advances</i> , 2021, 11, 38457-38472.	1.7	23
12316	Femtosecond photodecarbonylation of photo-ODIBO studied by stimulated Raman spectroscopy and density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25637-25648.	1.3	1
12317	The degradation effect on proton dissociation and transfer in perfluorosulfonic acid membranes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3007-3016.	1.3	3
12318	Diffusion Monte Carlo evaluation of disiloxane linearisation barrier. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	1.3	0
12319	Tuning the magnetic properties of a diamagnetic di-Blatter's zwitterion to antiferro- and ferromagnetically coupled diradicals. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2543-2553.	1.3	7
12320	Quantum chemistry study on the promoted reactivity of substituted cyclooctynes in bioorthogonal cycloaddition reactions. <i>Heterocyclic Communications</i> , 2021, 27, 142-154.	0.6	0
12321	CW/BSE nonadiabatic dynamics simulations on excited-state relaxation processes of zinc phthalocyanine-fullerene dyads: Roles of bridging chemical bonds. <i>Chinese Journal of Chemical Physics</i> , 2021, 34, 704-716.	0.6	5
12322	Reducing the reprocessing and healing temperature of polyurea with piperazine-based hindered urea bonds. <i>Materials Chemistry Frontiers</i> , 2022, 6, 473-481.	3.2	5
12323	Migration-assisted, moisture gradient process for ultrafast, continuous CO ₂ capture from dilute sources at ambient conditions. <i>Energy and Environmental Science</i> , 2022, 15, 680-692.	15.6	25
12324	Tris(Imidazolyl) Dicopper(I) Complex and its Reactivity to Exert Catalytic Oxidation of Sterically Hindered Phenol Substrates via a [Cu ₂ O] ²⁺ Core. <i>Dalton Transactions</i> , 2022, , .	1.6	0
12325	Thermodynamic Properties: Enthalpy, Entropy, Heat Capacity, and Bond Energies of Fluorinated Carboxylic Acids. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3-15.	1.1	5

#	ARTICLE	IF	CITATIONS
12326	Study of the variation of the optical properties of calcite with applied stress, useful for specific rock and material mechanics. <i>Scientific Reports</i> , 2022, 12, 299.	1.6	4
12327	Effects of methoxy group(s) on D- Γ -A porphyrin based DSSCs: efficiency enhanced by co-sensitization. <i>Materials Chemistry Frontiers</i> , 2022, 6, 580-592.	3.2	19
12328	Theoretical prediction of FNgM3 $\hat{=}$ kHk (Ng $\hat{=}$ Ar, Kr, Xe, and Rn; M $\hat{=}$ Cu, Ag and Au; k $\hat{=}$ O $\hat{=}$ 2) molecules. <i>Molecular Physics</i> , 0, , .	0.8	4
12329	Lactic acid photochemistry following excitation of S 0 to S 1 at 220 to 250 $\hat{=}$ nm. <i>Journal of Physical Organic Chemistry</i> , 0, , e4316.	0.9	3
12330	Linear fractional charge behavior in density functional theory through dielectric tuning of conductor-like polarizable continuum model. <i>Journal of Chemical Physics</i> , 2022, 156, 014106.	1.2	4
12331	Fundamental study on the selective etching of SiGe and Si in ClF3 gas for nanosheet gate-all-around transistor manufacturing: A first principle study. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , 2022, 40, .	0.6	2
12332	Surface modeling of photocatalytic materials for water splitting. <i>Physical Chemistry Chemical Physics</i> , 2021, , .	1.3	4
12333	Opportunities and challenges of applying advanced X-ray spectroscopy to actinide and lanthanide N-donor ligand systems. <i>Journal of Synchrotron Radiation</i> , 2022, 29, 53-66.	1.0	4
12334	Experimental and computational investigation of the bond energy of thorium dicarbonyl cation and theoretical elucidation of its isomerization mechanism to the thermodynamically most stable isomer, thorium oxide ketenylidene cation, OTh ⁺ CCO. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 842-853.	1.3	1
12335	NMR Coupling Constants Based on the Bethe $\hat{=}$ Salpeter Equation in the $\langle i \rangle$ GW $\langle /i \rangle$ Approximation. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1030-1045.	2.3	17
12336	Ruthenium complexes bearing N-heterocyclic carbene based CNC and CN [^] CHC [^] ™ pincer ligands: Photophysics, electrochemistry, and solar energy conversion. <i>Journal of Organometallic Chemistry</i> , 2022, 959, 122203.	0.8	6
12337	Adsorption of gas molecule on Rh, Ru doped monolayer MoS2 for gas sensing applications: A DFT study. <i>Chemical Physics Letters</i> , 2022, 789, 139300.	1.2	18
12338	High-performance symmetric supercapacitor based on new functionalized graphene oxide composites with pyrimidine nucleotide and nucleoside. <i>Journal of Molecular Liquids</i> , 2022, 348, 118381.	2.3	9
12339	Theoretical study of mechanisms and kinetics of reactions of the O(3P) atom with alkyl hydroperoxides (ROOH) where (R $\hat{=}$ CH3 & C2H5). <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113547.	1.1	2
12340	Recent advances in arsenene nanostructures towards prediction, properties, synthesis and applications. <i>Surfaces and Interfaces</i> , 2022, 28, 101610.	1.5	8
12341	Spectroscopic and computational studies of erythrosine food dye protonation in aqueous solution. <i>Dyes and Pigments</i> , 2022, 198, 110028.	2.0	12
12342	A mechanistic periodic DFT study on the dissociation of tetrachlorodibenzofuran (TCDF) by M-doped carbon nanotube catalysts (M $\hat{=}$ Al, Fe, Mn). <i>Applied Surface Science</i> , 2022, 579, 152217.	3.1	3
12343	Structural peculiarities of new benzopyrylium dyes: X-ray, FT-IR, and DFT complex study. <i>Journal of Molecular Structure</i> , 2022, 1252, 132178.	1.8	4

#	ARTICLE	IF	CITATIONS
12344	Aqueous zinc batteries using N-containing organic cathodes with Zn ²⁺ and H ⁺ Co-uptake. Chemical Engineering Journal, 2022, 431, 134253.	6.6	37
12345	Pharmacological and Molecular docking studies of new copper (II) complexes of N2-Phenyl-N4,N6-di(thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine. Journal of Molecular Structure, 2022, 1253, 132275.	1.8	4
12346	Cyanomethylation of 2,3,4,9-tetrahydro-1H-carbazol-1-one based on using two different reagents: Antioxidant activity and DFT studies. Journal of Molecular Structure, 2022, 1253, 132262.	1.8	0
12347	Cobalt(II), nickel(II), copper(II) and zinc(II) complexes of thiadiazole based Schiff base ligands: Synthesis, structural characterization, DFT, antidiabetic and molecular docking studies. Journal of Molecular Structure, 2022, 1253, 132266.	1.8	64
12348	Chemiluminescence emission in Fenton reaction driven by 1,2-dihydroxybenzenes: Mechanistic approaches using 4-substituted ligands. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 426, 113744.	2.0	0
12349	Manifestations of strong electron correlation in polyacene: Fundamental gap, density of states, and photoconductivity. Carbon Trends, 2022, 7, 100146.	1.4	3
12350	Synthesis of novel hybrid quinoxaline containing triazole and acetamide moieties by azide-alkyne click chemistry: Experimental and theoretical characterization. Journal of Molecular Structure, 2022, 1253, 132132.	1.8	18
12351	Interaction of simple amino acids (glycine, $\hat{1}$ -alanine, $\hat{2}$ -alanine and L-valine) with germatranol hydrate. Journal of Molecular Structure, 2022, 1253, 132245.	1.8	2
12352	Combined in situ XAS and DFT studies on the role of Pt in zeolite-supported metal catalysts for selective n-hexane isomerization. Fuel, 2022, 314, 123099.	3.4	7
12353	Surface molecule induced effective light absorption and charge transfer for H ₂ production photocatalysis in a carbonized polymer dots-carbon nitride system. Applied Catalysis B: Environmental, 2022, 305, 121064.	10.8	14
12354	Molecular simulations and experimental studies of the structural properties of imidazolium ionenes with butyl and decyl spacers solvated in 1-ethyl-3-methylimidazolium bistriflimide. Journal of Ionic Liquids, 2022, 2, 100013.	1.0	2
12355	Spectral, thermal and DFT studies of novel nickel(II) complexes of 2-benzoylpyridine-N4-methyl-3-thiosemicarbazone: Crystal structure of a square planar azido-nickel(II) complex. Journal of Molecular Structure, 2022, 1253, 132257.	1.8	10
12356	Organic materials based on thiophene and benzothiadiazole for organic solar cells. Computational investigations. , 2021, 5, .		1
12358	Organic Thermometers Based on Aggregation of Difluoroboron $\hat{2}$ -Diketonate Chromophores. Journal of Physical Chemistry A, 2020, 124, 10082-10089.	1.1	17
12360	KID Procedure Applied on the [(PY ₅ Me ₂)MoO] ⁺ Complex. ACS Omega, 2020, 5, 30549-30555.	1.6	2
12362	Adsorptive Complexation and Isotope Separation of Gadolinium Ion with Macrocyclic Crown Ether Embedded Polymeric Resin: Theory Guided Experiments. SSRN Electronic Journal, 0, , .	0.4	0
12363	Quantum chemical calculations of phenazine-based organic dyes in dye-sensitized solar cells. Heterocyclic Communications, 2021, 27, 155-163.	0.6	2
12364	Dipole Polarizability of C28 and its Counterparts Nb4B18 and Ta4B18. Insights from a Density Functional Theory (DFT) Endeavour. Journal of Physics: Conference Series, 2021, 2090, 012172.	0.3	0

#	ARTICLE	IF	CITATIONS
12365	COMPUTATIONAL INVESTIGATIONS, HIRSHFELD SURFACE ANALYSIS, INTERACTION ENERGY CALCULATIONS, AND ENERGY FRAMEWORK CRYSTAL STRUCTURE OF METHYL 2-AMINO-5-HYDROXYBENZOATE. <i>Journal of Structural Chemistry</i> , 2021, 62, 1745-1758.	0.3	1
12366	Investigation of the effect of surface phosphate ester dispersant on viscosity by coarse-grain modeling of BaTiO slurry. <i>Journal of the American Ceramic Society</i> , 2022, 105, 2791-2803.	1.9	0
12367	Transport mechanisms and desalination performance of the PSF/LiO-66 thin-film composite membrane: a molecular dynamics study. <i>Molecular Simulation</i> , 2022, 48, 427-437.	0.9	0
12368	Copper(II) Compounds of 4-Nitrobenzoic Hydrazide with Different Anions (ClO ₄ ⁻ , NO ₃ ⁻ and Br ⁻): Synthesis, Characterization, DFT calculations, DNA Interactions and Cytotoxic Properties. <i>Chemistry and Biodiversity</i> , 2022, , .	1.0	1
12369	Nitric oxide generation study of unsymmetrical 1 ² -diketiminato copper(II) nitrite complexes. <i>Dalton Transactions</i> , 2022, 51, 3485-3496.	1.6	7
12370	Unconventional mechanism and selectivity of the Pd-catalyzed C-H bond lactonization in aromatic carboxylic acid. <i>Nature Communications</i> , 2022, 13, 315.	5.8	8
12371	Mechanism unravelling for highly efficient and selective ⁹⁹ TcO ₄ ⁻ sequestration utilising crown ether based solvent system from nuclear liquid waste: experimental and computational investigations. <i>RSC Advances</i> , 2022, 12, 3216-3226.	1.7	9
12372	Synthesis, characterization, DFT calculations, and catalytic epoxidation of two oxovanadium(IV) Schiff base complexes. <i>Journal of the Turkish Chemical Society, Section A: Chemistry</i> , 0, , 163-208.	0.4	1
12373	Recent Advances in First-Principles Based Molecular Dynamics. <i>Accounts of Chemical Research</i> , 2022, 55, 221-230.	7.6	22
12374	Stable and inert macrocyclic cobalt(II) and nickel(II) complexes with paraCEST response. <i>Dalton Transactions</i> , 2022, 51, 1580-1593.	1.6	7
12375	Understanding the acrylates formation from CO ₂ and ethylene over Ni- and Pd-based catalysts: A DFT study on the effects of solvents, methyl halides, and ligands. <i>Molecular Catalysis</i> , 2022, 518, 112108.	1.0	2
12376	Ligand-protected gold nanoclusters probed by IRMPD spectroscopy and quantum chemistry calculations. <i>Journal of Molecular Spectroscopy</i> , 2022, 383, 111562.	0.4	1
12377	A chemical dynamics study of the reaction of the methylidyne radical (CH ₂ ⁺) with dimethylacetylene (CH ₃ CCCH ₃ , X ¹ A _{1g}). <i>Physical Chemistry Chemical Physics</i> , 2021, 24, 578-593.	1.3	12
12378	Unexpected discovery of estrone in the rotational spectrum of estradiol: a systematic investigation of a CP-FTMW spectrum. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 5539-5545.	1.3	2
12379	Hammett constants from density functional calculations: charge transfer and perturbations. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1.	0.5	7
12380	A Double-Site Chemodosimeter for Selective Fluorescence Detection of a Nerve Agent Mimic. <i>Molecules</i> , 2022, 27, 489.	1.7	8
12381	Concentration-dependent ion correlations impact the electrochemical behavior of calcium battery electrolytes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 674-686.	1.3	13
12382	Multireference Density Functional Theory for Describing Ground and Excited States with Renormalized Singles. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 894-903.	2.1	8

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12383	Cholesky decomposition of complex two-electron integrals over GIAOs: Efficient MP2 computations for large molecules in strong magnetic fields. <i>Journal of Chemical Physics</i> , 2022, 156, 044115.	1.2	17
12384	Formation of phenylacetylene and benzocyclobutadiene in the <i>ortho</i> -benzynes + acetylene reaction. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1869-1876.	1.3	4
12385	Ru-Catalyzed Enantioselective Hydrogenation of 2-Pyridyl-Substituted Alkenes and Substrate-Mediated H/D Exchange. <i>ACS Catalysis</i> , 2022, 12, 1150-1160.	5.5	8
12386	Computational insights into different regioselectivities in the Ir-porphyrin-catalyzed C-H insertion reaction of quinoid carbene. <i>Organic Chemistry Frontiers</i> , 2022, 9, 1143-1151.	2.3	2
12387	Solvent coordination to palladium can invert the selectivity of oxidative addition. <i>Chemical Science</i> , 2022, 13, 1618-1628.	3.7	12
12388	Demystifying constructive strategies on designing functionalized lamellar Nb ₂ CT _x nanosheet membrane architectures under confined space. <i>Journal of Materials Chemistry A</i> , 2022, 10, 4200-4208.	5.2	0
12389	In Situ XAFS, XRD, and DFT Characterization of the Sulfur Adsorption Sites on Cu and Ce Exchanged Y Zeolites. <i>Journal of Physical Chemistry C</i> , 2022, 126, 1496-1512.	1.5	8
12390	Comparison of green bio-based cerium/alginate vs. copper/alginate beads: a study of vibrational and thermal properties using experimental and theoretical methods. <i>Journal of Molecular Modeling</i> , 2022, 28, 37.	0.8	3
12391	Synthesis and Electronic Properties of Conjugated <i>syn</i> -Dithienothiazine Donor-Acceptor Donor Dumbbells. <i>European Journal of Organic Chemistry</i> , 2022, 2022, .	1.2	1
12392	LibSC: Library for Scaling Correction Methods in Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 840-850.	2.3	8
12393	New N,N'-bis(thioamido)thiocarbohydrazones and carbohydrazones: synthesis, structure characterization, antioxidant activity, corrosion inhibitors and DFT studies. <i>Research on Chemical Intermediates</i> , 2022, 48, 1593-1613.	1.3	10
12394	Modification of the Second Harmonic Generation and Fluorescence Efficiency of D289 Dye Based on a Donor-Acceptor Structure. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2234-2242.	1.5	6
12395	Synthesis and evaluation of potent yaku'amide A analogs. <i>Chemical Science</i> , 2022, 13, 1899-1905.	3.7	1
12396	Mechanism and selectivity of photocatalyzed CO ₂ reduction by a function-integrated Ru catalyst. <i>Dalton Transactions</i> , 2022, 51, 3747-3759.	1.6	4
12397	Lacking of ESIPT Band of Aromatic <i>ortho</i> -Aminoaldehyde Derivatives Triggered by the N-H Vibration. <i>Physical Chemistry Chemical Physics</i> , 2022, .	1.3	0
12398	The Mechanism and Kinetics Model of Degradation of Dicarboxylic Acids by Hydroxyl Radicals under Atmospheric Conditions. <i>Journal of Physical Chemistry A</i> , 2022, 126, 787-799.	1.1	1
12399	The Second Excited Triplet State Facilitates TADF and Triplet-Triplet Annihilation Photon Upconversion via a Thermally Activated Reverse Internal Conversion. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	7
12400	Defect-Induced π -Magnetism into Non-Benzenoid Nanographenes. <i>Nanomaterials</i> , 2022, 12, 224.	1.9	7

#	ARTICLE	IF	CITATIONS
12401	Understanding the Effect of pH on the Solubility and Aggregation Extent of Humic Acid in Solution by Combining Simulation and the Experiment. <i>Environmental Science & Technology</i> , 2022, 56, 917-927.	4.6	35
12402	Preparation of Luminescent Plasmonic Silver Nanoparticles for Electrochemical Detection of Sulphide and Thiourea in Aqueous Solution and Ab Initio DFT Study of the Chemical Affinity Towards Silver Nanoparticles. <i>Plasmonics</i> , 2022, 17, 1017-1024.	1.8	3
12403	Investigation of the Coordination Chemistry of a Bisamidinate Ferrocene Ligand with Cu, Ag, and Au. <i>ACS Omega</i> , 2022, 7, 4683-4693.	1.6	1
12404	Revisiting Solvent-Dependent Roles of the Electrolyte Counteranion in O_2 Batteries upon CO_2 Incorporation. <i>ACS Applied Energy Materials</i> , 2022, 5, 2150-2160.	2.5	4
12405	Nitrene formation is the first step of the thermal and photochemical decomposition reactions of organic azides. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 5109-5115.	1.3	17
12406	Unravelling the origin of dual photoluminescence in Au_2Cu_6 clusters by triplet sensitization and photon upconversion. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4597-4606.	2.7	8
12407	Accurate predictions of the electronic excited states of BODIPY based dye sensitizers using spin-component-scaled double-hybrid functionals: a TD-DFT benchmark study. <i>RSC Advances</i> , 2022, 12, 1704-1717.	1.7	11
12408	Theoretical studies on the two-photon absorption of VI semiconductor nano clusters. <i>Scientific Reports</i> , 2022, 12, 110.	1.6	3
12409	Automatic Approach to Explore the Multireaction Mechanism for Medium-Sized Bimolecular Reactions via Collision Dynamics Simulations and Transition State Searches. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 910-924.	2.3	6
12410	Ultrafast carrier dynamics at organic donor-acceptor interfaces: a quantum-based assessment of the hopping model. <i>JPhys Materials</i> , 2022, 5, 024001.	1.8	6
12411	Unraveling the Mechanism of Palladium-Catalyzed Base-Free Cross-Coupling of Vinyl Carboxylates: Dual Role of Arylboronic Acids as a Reducing Agent and a Coupling Partner. <i>ACS Catalysis</i> , 2022, 12, 1809-1817.	5.5	3
12412	The predicted models of anti-colon cancer and anti-hepatoma activities of substituted 4-anilino coumarin derivatives using quantitative structure-activity relationship (QSAR). <i>Journal of King Saud University - Science</i> , 2022, 34, 101837.	1.6	3
12413	Mechanism of Diiron Hydrogenase Complexes Controlled by Nature of Bridging Dithiolate Ligand. <i>ChemistryOpen</i> , 2022, 11, e202100238.	0.9	6
12414	Local Electronic Charge Transfer in the Helical Induction of Cis-Transoid Poly(4-carboxyphenyl)acetylene by Chiral Amines. <i>Journal of Chemical Information and Modeling</i> , 2022, , .	2.5	1
12415	Enantiopure, luminescent, cyclometalated Ir(III) complexes with N-heterocyclic carbene-naphthalimide chromophore: design, vibrational circular dichroism and TD-DFT calculations. <i>Dalton Transactions</i> , 2022, , .	1.6	10
12416	En Synthesis of a Pentabenzopentaaza[10]circulene. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	14
12417	En Synthesis of a Pentabenzopentaaza[10]circulene. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	4
12418	Electrochemical Water Splitting: H_2 Evolution Reaction. <i>Materials Horizons</i> , 2022, , 59-89.	0.3	2

#	ARTICLE	IF	CITATIONS
12419	Nucleophilicity and Electrophilicity in the Gas Phase: Silane Hydricity. <i>Journal of Organic Chemistry</i> , 2022, 87, 1840-1849.	1.7	2
12420	Theoretical studies on the proton dissociation and degradation of sulfonated polyethylene electrolyte membrane. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 5553-5563.	3.8	0
12421	Sc doped WSe ₂ monolayer: a candidate for enhanced adsorption and detection of SF ₆ decomposition gases. <i>Journal of Materials Research and Technology</i> , 2022, 17, 1786-1798.	2.6	7
12422	Elucidating the mechanism and reactivity of the reaction between the donor-acceptor 1,3-bis(diazo) compound and cinnamyl alcohol catalyzed by Rh ₂ (OAc) ₄ : a DFT study. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
12423	Triplet-Triplet Annihilation Upconversion from Ru(II) Phenanthroline Complexes and Substituted Anthracene Derivatives. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0
12424	Study of chemical, kinetic, and theoretical sorption properties of activated carbons obtained from agroindustrial origin: comparison of anionic and cationic model molecules. <i>Biomass Conversion and Biorefinery</i> , 2024, 14, 733-750.	2.9	4
12425	DFT study of the influence of boron/nitrogen substitution on the electronic and nonlinear optical properties of the benzene-substituted graphdiyne fragment. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113629.	1.1	4
12426	Mechanistic Investigation of H ₂ O ₂ -dependent Chemiluminescence from Tetrabromo-1,4-Benzoquinone. <i>ChemPhysChem</i> , 2022, 23, e202100885.	1.0	3
12427	Synthesis, spectroscopic characterization of new series of alizarin derivatives and their anti-microbial activities: DFT and molecular docking approach. <i>Journal of Molecular Structure</i> , 2022, 1256, 132527.	1.8	2
12428	Thermodynamically Favourable States in the Reaction of Nitrogenase without Dissociation of any Sulfide Ligand. <i>Chemistry - A European Journal</i> , 2022, , .	1.7	12
12429	Ester-Carbene and Its Dimerization with Exclusive Cis-Selectivity on a Silver Surface. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2482-2492.	1.5	0
12430	<i>in silico</i> Analysis of Aldofuranosyl Rings: Unbiased Modeling of Conformational Equilibria and Dynamics in Solution. <i>Biochemistry</i> , 2022, 61, 239-251.	1.2	6
12431	Ab initio and DFT benchmark study for the calculations of isotopic shifts of fundamental frequencies for 2,3-dihydropyran. <i>Structural Chemistry</i> , 0, , 1.	1.0	1
12432	Composites of porous materials with ionic liquids: Synthesis, characterization, applications, and beyond. <i>Microporous and Mesoporous Materials</i> , 2022, 332, 111703.	2.2	30
12433	Dynamic toroidizability as ubiquitous property of atoms and molecules in optical electric fields. <i>Journal of Chemical Physics</i> , 2022, 156, 054106.	1.2	6
12434	Olefin oligomerization by zirconium boratabenzene catalysts. <i>Journal of Organometallic Chemistry</i> , 2022, 962, 122268.	0.8	0
12435	Predicting the reactivity of unsaturated molecules to methyl radical addition using a radical two-parameter general-purpose reactivity indicator. <i>Chemical Physics Letters</i> , 2022, 791, 139333.	1.2	4
12436	Electronic and optical properties of ultra-small diameter armchair carbon and boron nitride nanotubes by PBE, TB-mBJ and YS-PBE0 functionals. <i>Diamond and Related Materials</i> , 2022, 123, 108863.	1.8	11

#	ARTICLE	IF	CITATIONS
12437	Calculation of vertical and adiabatic ionization potentials for some benzaldehydes using hybrid DFT, multilevel G3B3 and MP2 methods. <i>Chemical Physics Letters</i> , 2022, 791, 139349.	1.2	18
12438	Photoactivated Ru chemical vapor deposition using (η^3 -allyl)Ru(CO)3X (X = Cl, Br, I): From molecular adsorption to Ru thin film deposition. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2022, 40, 023404.	0.9	1
12439	Chromone derived effective probe for the detection of metal ion (Cu ²⁺) and chemical explosive (p-nitrotoluene). <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 427, 113823.	2.0	6
12440	γ -Ag ₂ WO ₄ under microwave, electron beam and femtosecond laser irradiations: Unveiling the relationship between morphology and photoluminescence emissions. <i>Journal of Alloys and Compounds</i> , 2022, 903, 163840.	2.8	3
12441	Simulation of the Physicochemical Properties of Anatase TiO ₂ with Oxygen Vacancies and Doping of Different Elements for Photocatalysis Processes. <i>Lecture Notes in Networks and Systems</i> , 2022, , 238-249.	0.5	0
12442	Dehydrogenation of formic acid using iridium-NSi species as catalyst precursors. <i>Dalton Transactions</i> , 2022, 51, 4386-4393.	1.6	8
12443	Palladium-catalyzed selective C=C bond cleavage and stereoselective alkenylation between cyclopropanol and 1,3-diyne: one-step synthesis of diverse conjugated enynes. <i>Chemical Science</i> , 2022, 13, 2692-2700.	3.7	17
12444	Nonlinear activity and long-term stability of thin polymer films based on poly(3,5,7,3,4-pentahydroxyflavone-8-sulfonic acid) sodium salt. <i>Polymers and Polymer Composites</i> , 2022, 30, 096739112110729.	1.0	0
12445	Quantum-chemical studies of the antioxidant effectiveness of <i>p</i> -phenylene diamines. <i>Journal of Vinyl and Additive Technology</i> , 2022, 28, 352-366.	1.8	3
12446	In silico design of novel anticancer drugs with amino acid and carbohydrate building blocks to inhibit PIM kinases. <i>Molecular Simulation</i> , 0, , 1-15.	0.9	0
12447	Adiabatic Connection for Range-Separated Hybrid Functionals. <i>Advanced Theory and Simulations</i> , 2022, 5, .	1.3	1
12448	Ru(0)-Catalyzed Regioselective Synthesis of Borylated-1,4- and -1,5-Diene Building Blocks. <i>Organometallics</i> , 2022, 41, 390-411.	1.1	1
12449	Stereoselective, Ruthenium-Photocatalyzed Synthesis of 1,2-Diaminotruxinic Bis-amino Acids from 4-Arylidene-5(4H)-oxazolones. <i>Journal of Organic Chemistry</i> , 2022, , .	1.7	6
12450	Sensitivity of the electronic and magnetic structures of cuprate superconductors to density functional approximations. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	12
12451	Counterintuitive Electrostatics upon Metal Ion Coordination to a Receptor with Two Homotopic Binding Sites. <i>Journal of the American Chemical Society</i> , 2022, 144, 2921-2932.	6.6	3
12452	Free Energy Profiles of Proton Transfer Reactions: Density Functional Benchmark from Biased Ab Initio Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2022, , .	2.3	5
12453	Synthesis of thiophene derivatives: Substituent effect, antioxidant activity, cyclic voltammetry, molecular docking, DFT, and TD-DFT calculations. <i>Journal of Molecular Structure</i> , 2022, 1257, 132607.	1.8	14
12454	Experimental and Theoretical Studies of Trans-2-Pentenal Atmospheric Ozonolysis. <i>Atmosphere</i> , 2022, 13, 291.	1.0	1

#	ARTICLE	IF	CITATIONS
12455	Key Piece in the Wolfe Cycle of Methanogenesis: The S–S Bond Dissociation Conducted by Noncubane [Fe ₄ S ₄] Cluster-Dependent Heterodisulfide Reductase. <i>ACS Catalysis</i> , 2022, 12, 2606-2622.	5.5	3
12456	The Role of Hydrogen Bonds and Electrostatic Interactions in Enhancing Two-Photon Absorption in Green and Yellow Fluorescent Proteins. <i>ChemPhysChem</i> , 2022, 23, .	1.0	4
12457	One-Step Synthesis of novel N1 -substituted benzimidazole derivatives: Experimental and theoretical investigations. <i>Journal of Heterocyclic Chemistry</i> , 0, , .	1.4	3
12458	A general justification for hybrid functionals in DFT by means of linear response theory*. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 194004.	0.7	0
12459	Assembling of Perylene, Naphthalene, and Pyromellitic Diimide-Based Materials and Their Third-Order Nonlinear Optical Properties. <i>Journal of Physical Chemistry A</i> , 2022, 126, 870-878.	1.1	8
12460	Discover, Sample, and Refine: Exploring Chemistry with Enhanced Sampling Techniques. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1424-1430.	2.1	12
12461	Improving Density Functional Prediction of Molecular Thermochemical Properties with a Machine-Learning-Corrected Generalized Gradient Approximation. <i>Journal of Physical Chemistry A</i> , 2022, 126, 970-978.	1.1	4
12462	Coordination of new palladium (II) complexes with derived furofuran-3,4-dione ligands: Synthesis, characterization, redox behaviour, DFT, antimicrobial activity, molecular docking and ADMET studies. <i>Journal of Molecular Structure</i> , 2022, 1257, 132611.	1.8	11
12463	Spirovetivane- and Eudesmane-Type Sesquiterpenoids Isolated from the Culture Media of Two Cyanobacterial Strains. <i>Journal of Natural Products</i> , 2022, 85, 415-425.	1.5	2
12464	Molecular Geometry Dependent Electronic Coupling and Reorganization Energy for Electron Transfer between Dye Molecule Adsorbed on TiO ₂ Electrode and Co Complex in Electrolyte Solutions. <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	2
12465	Innovative characterization of original green vanillin-derived Schiff bases as corrosion inhibitors by a synergic approach based on electrochemistry, microstructure, and computational analyses. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 641, 128540.	2.3	24
12466	Synthesis, structural elucidation, DFT calculation, biological studies and DNA interaction of some aryl hydrazone Cr ³⁺ , Fe ³⁺ , and Cu ²⁺ chelates. <i>Computational Biology and Chemistry</i> , 2022, 97, 107643.	1.1	66
12467	β-Cyclodextrin capped silver and gold nanoparticles as colorimetric and Raman sensor for detecting traces of pesticide -Chlorpyrifos- in fruits and vegetables. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 641, 128558.	2.3	13
12468	Charge scaling parameter evaluation for multivalent ionic liquids with fixed point charge force fields. <i>Journal of Ionic Liquids</i> , 2022, 2, 100020.	1.0	8
12469	Synthesis and Computational Characterization of Organic UV-Dyes for Cosensitization of Transparent Dye-Sensitized Solar Cells. <i>Molecules</i> , 2021, 26, 7336.	1.7	4
12470	Hyperfine Coupling Constants in Local Exact Two-Component Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 323-343.	2.3	15
12471	A Comparison of Exact and Model Exchange–Correlation Potentials for Molecules. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 12012-12019.	2.1	13
12472	Subnano-sized silicon anode via crystal growth inhibition mechanism and its application in a prototype battery pack. <i>Nature Energy</i> , 2021, 6, 1164-1175.	19.8	107

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12473	Investigation on micro-mechanism of palm oil as natural ester insulating oil for overheating thermal fault analysis of transformers. High Voltage, 2022, 7, 812-824.	2.7	20
12474	Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585.		0
12475	Dft Study on the Mechanism of the Co ₂ -to-Co Conversion by Co-Quaterpyridine Complex. SSRN Electronic Journal, 0, , .	0.4	0
12476	Dft Investigation on Two Dimensional ZnO/MoSe ₂ Van Der Waals Heterostructures as Promising Photocatalysts for Hydrogen Production. SSRN Electronic Journal, 0, , .	0.4	0
12477	Synthesis of the β -dipyrrinyl triphyrin(2.1.1) ligand and its coordination complexes. Dalton Transactions, 2022, 51, 6399-6409.	1.6	3
12478	Benchmarks of the density functional tight-binding method for redox, protonation and electronic properties of quinones. Physical Chemistry Chemical Physics, 2022, 24, 6742-6756.	1.3	0
12479	First Order Hyper polarizability and Intramolecular Charge Transfer of N-Ethyl-N-(2-Hydroxyethyl)-4-(4-Nitrophenylazo) Aniline for Photonic Applications. IOP Conference Series: Materials Science and Engineering, 2022, 1219, 012035.	0.3	1
12480	Assessment of time-dependent density functionals for the electronic excitation energies of organic dyes used in DSSCs. New Journal of Chemistry, 2022, 46, 7682-7694.	1.4	7
12481	A review of atomic layer deposition modelling and simulation methodologies: Density functional theory and molecular dynamics. Nanotechnology Reviews, 2022, 11, 1332-1363.	2.6	20
12482	Computational and Experimental Study of Different Brines in Temperature Swing Solvent Extraction Desalination with Amine Solvents. SSRN Electronic Journal, 0, , .	0.4	0
12483	Competitive Adsorption of Anionic and Cationic Molecules on Three Activated Carbons Derived from Agroindustrial Waste. SSRN Electronic Journal, 0, , .	0.4	1
12484	Dft Investigation on Two Dimensional ZnO/MoSe ₂ Van Der Waals Heterostructures as Promising Photocatalysts for Hydrogen Production. SSRN Electronic Journal, 0, , .	0.4	0
12486	Towards custom built double core carbon nanothreads using stilbene and pseudo-stilbene type systems. Nanoscale, 2022, 14, 4614-4625.	2.8	11
12487	Dft Investigation on Two Dimensional ZnO/MoSe ₂ Van Der Waals Heterostructures as Promising Photocatalysts for Hydrogen Production. SSRN Electronic Journal, 0, , .	0.4	0
12488	Theoretical investigation of the β -substitution effect on β -C(sp ³)-H arylation of amines: structure-reactivity relationship (SRR) studies. Organic Chemistry Frontiers, 0, , .	2.3	0
12489	Poisoning density functional theory with benchmark sets of difficult systems. Physical Chemistry Chemical Physics, 2022, 24, 6398-6403.	1.3	12
12490	Investigation of W/Mo Co-Doping with Multiple Concentrations in Photocatalyst BiVO ₄ By First-Principles Calculations. SSRN Electronic Journal, 0, , .	0.4	0
12491	Pu(III) and Cm(III) in the presence of EDTA: aqueous speciation, redox behavior, and the impact of Ca(II). RSC Advances, 2022, 12, 9478-9493.	1.7	2

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12492	Mechanistic exploration of CO ₂ conversion to dimethoxymethane (DMM) using transition metal (Co, Ru) catalysts: an energy span model. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8387-8397.	1.3	9
12493	Computational development of a phase-sensitive membrane raft probe. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8260-8268.	1.3	1
12494	Structural and electronic properties for Be-doped Pt _n (<i>n</i> = 1–12) clusters obtained by DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7856-7861.	1.3	4
12495	Copper(II) Chelates Derived from an N,N,O-Tridentate 2-Pyridinecarboxaldehyde-N4-Phenylsemicarbazone: Synthesis, Spectral Aspects, Fmo and Nbo Analysis. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12496	Effects of Non-Local Exchange Functionals in the Density Functional Theories for the Description of Molecular Vibrations. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12497	Stability-Order Reversal in FSiY and FYSi (Y = N and P) Molecules after the Insertion of a Noble Gas Atom. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1132-1143.	1.1	4
12498	Design of a manufactured organic dye molecules with different spacers for highly efficient reliable DSSCs via computational analysis. <i>Molecular Simulation</i> , 2022, 48, 584-593.	0.9	2
12499	Structural and Dynamic Disorder, Not Ionic Trapping, Controls Charge Transport in Highly Doped Conducting Polymers. <i>Journal of the American Chemical Society</i> , 2022, 144, 3005-3019.	6.6	45
12500	2,7-Substituted <i>N</i> -Carbazole Donors on Tris(2,4,6-trichlorophenyl)methyl Radicals with High Quantum Yield. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	15
12501	Evaluation of OH Radical Reaction Positions in 3-Ring PAHs Using Transition State Energy and Atomic Charge Calculations. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 2479.	1.3	2
12502	The Potential Energy Profile of the HBr ⁺ + HCl Bimolecular Collision. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1465-1474.	1.1	4
12503	Free Energy and Stacking of Eumelanin Nanoaggregates. <i>Journal of Physical Chemistry B</i> , 2022, 126, 1805-1818.	1.2	8
12504	Computational characterization of nanosystems. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 1-15.	0.6	2
12505	Insights from Density Functional Theory on the Feasibility of Modified Reactive Dyes as Dye Sensitizers in Dye-Sensitized Solar Cell Applications. <i>Solar</i> , 2022, 2, 12-31.	0.9	16
12506	<i>Saturnenes</i> Like Th@Au ₆ D _{6h} : Ring-Current Evidence for Au ⁺ Au Bonding Along the Gold Ring. <i>Israel Journal of Chemistry</i> , 2022, 62, .	1.0	2
12507	Analysis of the Geometric and Electronic Structure of Spin-Coupled Iron-Sulfur Dimers with Broken-Symmetry DFT: Implications for FeMoco. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1437-1457.	2.3	16
12508	Determination of two-photon absorption in nucleobase analogues: a QR-DFT perspective. <i>Photochemical and Photobiological Sciences</i> , 2022, , 1.	1.6	0
12509	Photodegradation of Congo Red by Modified P25-Titanium Dioxide with Cobalt-Carbon Supported on SiO ₂ Matrix, DFT Studies of Chemical Reactivity. <i>Catalysts</i> , 2022, 12, 248.	1.6	6

#	ARTICLE	IF	CITATIONS
12510	BN-Substitution in Dithienylpyrenes Prevents Excimer Formation in Solution and in the Solid State. <i>Journal of Physical Chemistry C</i> , 2022, 126, 4563-4576.	1.5	5
12511	Bis-(Fluorene)-Embedded Hexaphyrins. <i>Journal of Organic Chemistry</i> , 2022, 87, 2543-2550.	1.7	5
12512	All-Solid-State Vertical Three-Terminal N-Type Organic Synaptic Devices for Neuromorphic Computing. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	28
12513	Antimalarial Activity of Highly Coordinative Fused Heterocycles Targeting \hat{I}^2 Hematin Crystallization. <i>ACS Omega</i> , 2022, 7, 7499-7514.	1.6	10
12514	Generalized energy-based fragmentation approach for accurate binding energies and Raman spectra of methane hydrate clusters. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 167-176.	0.6	3
12515	Tunable Fluorescence and Afterglow in Organic Crystals for Temperature Sensing. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1985-1990.	2.1	18
12516	High-Pressure Synthesis of 1D Low-Bandgap Polymers Embedded in Diamond-like Carbon Nanothreads. <i>Chemistry of Materials</i> , 2022, 34, 2422-2428.	3.2	13
12517	Design of a D- π -A-A framework with various auxiliary acceptors on optoelectronic and charge transfer properties for efficient dyes in DSSCs: A DFT/TD-DFT study. <i>Journal of Computational Electronics</i> , 2022, 21, 361-377.	1.3	1
12518	Electron-spin interaction in the spin-Peierls phase of the organic spin chain (T_j ETQq0 0.0 rgBT /Overlock 10 Tf 50 442 Td)	1.1	4
12519	Physical Review B, 2022, 105, . Cosolvent Effect on the Solubility of Ammonium Benzoate in Supercritical Carbon Dioxide. <i>Journal of Chemical & Engineering Data</i> , 2022, 67, 689-694.	1.0	4
12520	Second-Order Active-Space Embedding Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1527-1541.	2.3	6
12521	Synthesis of Pyridine-Containing Crowned Fused Expanded Porphyrins. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	6
12522	Topical Anti-Inflammatory Activity of <i>Petiveria alliacea</i> , Chemical Profiling and Computational Investigation of Phytoconstituents Identified from its Active Fraction. <i>Chemistry Africa</i> , 2022, 5, 557-565.	1.2	5
12523	Quasi-Relativistic Calculation of EPR g Tensors with Derivatives of the Decoupling Transformation, Gauge-Including Atomic Orbitals, and Magnetic Balance. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2246-2266.	2.3	16
12524	Quantum chemical and photophysical properties of 9-Chloro 2, 6-Dimethyl 10(Methylsulfanyl)Quinoxaline. <i>Materials Today: Proceedings</i> , 2022, , .	0.9	0
12525	The Two Hot Corinos of the SVS13-A Protostellar Binary System: Counterposed Siblings. <i>Astrophysical Journal Letters</i> , 2022, 928, L3.	3.0	15
12526	Facile One-Pot Multi-Component Synthesis, Characterization, Molecular Docking Studies, Biological Evaluation of 1,2,4-Triazolo Isoindoline-1,3-Diones and Their DFT Calculations. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 2283-2301.	1.4	1
12527	Magnetic Characterization of Open-Shell Donor-Acceptor Conjugated Polymers. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5701-5710.	1.5	9

#	ARTICLE	IF	CITATIONS
12528	A DFT study on the reaction mechanisms of the oxidation of ethylene mediated by technetium and manganese oxo complexes. <i>Journal of Molecular Modeling</i> , 2022, 28, 94.	0.8	2
12529	Quantum Mechanical Simulations of the Radicalâ€“Radical Chemistry on Icy Surfaces. <i>Astrophysical Journal, Supplement Series</i> , 2022, 259, 39.	3.0	24
12530	Rotational Spectrum and Conformational Analysis of Perillartine: Insights into the Structureâ€“Sweetness Relationship. <i>Molecules</i> , 2022, 27, 1924.	1.7	1
12531	Mechanisms of Strain-Induced Interfacial Strengthening of Wet-Spun Filaments. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 16809-16819.	4.0	5
12532	Classical nuclear motion: Does it fail to explain reactions and spectra in certain cases?. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	2
12533	Single Excitation Energies Obtained from the Ensemble â€œHOMOâ€“LUMO Gapâ€“ Exact Results and Approximations. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2452-2458.	2.1	14
12534	Theoretical Modeling of Absorption and Fluorescent Characteristics of Cyanine Dyes. <i>Photochem</i> , 2022, 2, 202-216.	1.3	5
12535	Hyper-CEST NMR of metal organic polyhedral cages reveals hidden diastereomers with diverse guest exchange kinetics. <i>Nature Communications</i> , 2022, 13, 1708.	5.8	20
12536	Structural, Spectroscopic, NBO and Molecular Docking Analysis of 5-Nitrobenzimidazole â€“ A DFT Approach. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 2889-2907.	1.4	4
12537	Theoretical evidence for the formation of perfluorocarboxylic acids from atmospheric oxidation degradation of fluorotelomer acrylates. <i>Environmental Science and Pollution Research</i> , 2022, 29, 55092-55104.	2.7	1
12538	Relativistic Effects in Modeling the Ligand K-Edge X-ray Absorption Near-Edge Structure of Uranium Complexes. <i>Journal of Chemical Theory and Computation</i> , 2022, .	2.3	3
12539	The effect of <sc>off-center</sc> ĩf-hole on the <sc>atom-centered</sc> partial charges in halogenated molecules. <i>Journal of Computational Chemistry</i> , 2022, 43, 864-869.	1.5	0
12540	Consecutive Threeâ€“component Synthesis of Phenothiazine Based Merocyanines â€“ Bayesian Optimization, Electronic properties, and DSSC Characteristics. <i>European Journal of Organic Chemistry</i> , 0, .	1.2	2
12541	EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory. <i>Magnetochemistry</i> , 2022, 8, 36.	1.0	7
12542	Dielectric-Optical Switches: Photoluminescent, EPR, and Magnetic Studies on Organicâ€“Inorganic Hybrid (azetidinium)₂MnBr₄. <i>Inorganic Chemistry</i> , 2022, 61, 5626-5636.	1.9	20
12543	Barrier Potential, Structure (Monomer and Dimer), Inter- and Intra-Molecular Interactions, Vibrational Analysis, Fukui Functions, MESP, NBO, UV and NMR Analysis of Pyridine-3-Carboxylic Acid Using Spectroscopic and DFT Approach. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 2488-2505.	1.4	8
12544	Origin independent current density vector fields induced by time-dependent magnetic field. I. The LiH molecule. <i>Journal of Chemical Physics</i> , 2022, 156, 154105.	1.2	6
12545	Mechanical strength and band alignment of BAs/GaN heterojunction polar interfaces: A first-principles calculation study. <i>Physical Review Materials</i> , 2022, 6, .	0.9	2

#	ARTICLE	IF	CITATIONS
12546	Molybdenum bound nitrogen-doped graphene catalyst for reduction of N ₂ to NH ₃ and NH ₂ NH ₂ , using FLP as a co-catalyst: A DFT study. Applied Organometallic Chemistry, 0, .	1.7	3
12547	Fragmentation inside proton-transfer-reaction-based mass spectrometers limits the detection of ROOR and ROOH peroxides. Atmospheric Measurement Techniques, 2022, 15, 1811-1827.	1.2	14
12548	First-principles Study on Equilibrium Sn Isotope Fractionations in Hydrothermal Fluids. Acta Geologica Sinica, 2022, 96, 2125-2134.	0.8	2
12549	Fast All-Electron Hybrid Functionals and Their Application to Rare-Earth Iron Garnets. Frontiers in Materials, 2022, 9, .	1.2	1
12550	Combining Localized Orbital Scaling Correction and Bethe-Salpeter Equation for Accurate Excitation Energies. Journal of Chemical Physics, 2022, 156, 154101.	1.2	6
12551	Photochemistry of (η^4 -diene)Ru(CO) ₃ Complexes as Precursor Candidates for Photoassisted Chemical Vapor Deposition. Organometallics, 2022, 41, 761-775.	1.1	2
12552	Non-energetic Formation of Ethanol via CCH Reaction with Interstellar H ₂ O Ices. A Computational Chemistry Study. ACS Earth and Space Chemistry, 2022, 6, 496-511.	1.2	19
12553	Isolation, Identification, and DFT-Based Conformational Analysis of Sesquikarahanadienone and Its Congeners from Freshwater Dothideomycetes <i>Neohelicascus Aquaticus</i> KT4120. Bulletin of the Chemical Society of Japan, 2022, 95, 833-845.	2.0	4
12554	Gas-phase experimental and computational studies of human hypoxanthine-guanine phosphoribosyltransferase substrates: Intrinsic properties and biological implications. Journal of Physical Organic Chemistry, 2022, 35, .	0.9	3
12555	Highly Effective Activated Carbon-Supported Ni-Mn Bifunctional Catalyst for Selective Hydrodeoxygenation of 5-Hydroxymethylfurfural to 2,5-Dimethylfuran. ChemSusChem, 2022, 15, .	3.6	4
12556	Hubbard-corrected oxide formation enthalpies without adjustable parameters. Journal of Physics Communications, 2022, 6, 035009.	0.5	5
12557	High Fe utilization efficiency and low toxicity of Fe ₃ C@FeO loaded biochar for removing of tetracycline hydrochloride in wastewater. Journal of Cleaner Production, 2022, 353, 131630.	4.6	18
12558	Effects of auxiliary electron-withdrawing moieties on the photovoltaic properties of D- π -A TM - π -A phosphonic acid-based DSSCs. Computational and Theoretical Chemistry, 2022, 1210, 113645.	1.1	6
12559	A DFT study on the mechanism of NO and N ₂ O decomposition catalysed by Cu(I) pairs in Cu-ZSM-5: Revisited reactivity at the M6 ring. Molecular Catalysis, 2022, 522, 112206.	1.0	0
12560	On the nature of decoherence in quantum circuits: Revealing the structural motif of the surface radicals in \pm -Al ₂ O ₃ . Science Advances, 2022, 8, eabm6169.	4.7	5
12561	Deep dive into machine learning density functional theory for materials science and chemistry. Physical Review Materials, 2022, 6, .	0.9	28
12562	Losartan Interactions with 2-Hydroxypropyl- β -CD. Molecules, 2022, 27, 2421.	1.7	4
12563	Hybrid DFT small-cluster model of CO oxidation on CeO ₂ (110). Chemical Physics Letters, 2022, 793, 139436.	1.2	3

#	ARTICLE	IF	CITATIONS
12564	Optimal Tuning Perspective of Range-Separated Double Hybrid Functionals. Journal of Chemical Theory and Computation, 2022, 18, 2331-2340.	2.3	6
12565	Evaluation of the Adsorptive Potential of Zeolite Volcanic Tuff in Single and Binary Aqueous Solutions of the Basic Blue 41 Cationic Dye. ChemistrySelect, 2022, 7, .	0.7	1
12566	A Tip-Inhibitor Interphase Embedded with Soluble Polysulfides for High-Voltage Li Metal Batteries. Energy and Environmental Materials, 2023, 6, .	7.3	2
12567	Metallocene-incorporated Hybrid Singly N-Methyl-Confused Calixphyrins: Synthesis, Characterization, Protonation and Deprotonation Studies. Chemistry - an Asian Journal, 2022, 17, .	1.7	1
12568	A combined experimental-computational approach for electrocatalytic detection of epinephrine using nanocomposite sensor based on polyaniline/nickel oxide. Journal of Electroanalytical Chemistry, 2022, 911, 116204.	1.9	3
12569	A CobaltII/CobaltIII complex of alizarin that was analyzed from the stand point of binding with DNA, for ROS generation and anticancer drug prospecting was identified as an analogue of anthracyclines. Journal of Molecular Structure, 2022, 1262, 133011.	1.8	2
12570	Transient uniform electron gases. Molecular Physics, 2023, 121, .	0.8	0
12571	Synthesis, spectroscopic, CO-releasing ability, and anticancer activity studies of [Mn(CO) ₃ (L)Br] complexes: Experimental and density functional theory studies. Applied Organometallic Chemistry, 2022, 36, .	1.7	4
12572	Theoretical study of magnetic phase transition in La ₂ VO ₄ . Physics Letters, Section A: General, Atomic and Solid State Physics, 2022, 432, 128010.	0.9	0
12573	Many Body Current Density from Foldy-Wouthuysen Transformation of the Dirac-Coulomb Hamiltonian. Physchem, 2022, 2, 96-107.	0.5	1
12574	Experimental and theoretical approaches on structural, spectroscopic (FT-IR and UV-Vis), nonlinear optical, and molecular docking analyses for Zn (II) and Cu (II) complexes of 6-chloropyridine-2-carboxylic acid. Applied Organometallic Chemistry, 2022, 36, .	1.7	10
12575	Improving Results by Improving Densities: Density-Corrected Density Functional Theory. Journal of the American Chemical Society, 2022, 144, 6625-6639.	6.6	45
12576	Enantioselective Cytotoxicity of Chiral Diphosphine Ruthenium(II) Complexes Against Cancer Cells. Chemistry - A European Journal, 2022, , .	1.7	7
12577	Ring-opening polymerization of Lactide catalyzed by food sweetener saccharin with organic base mediated: A computational study. Polymer, 2022, 246, 124747.	1.8	3
12578	Effect of Electron Donating/Withdrawing Groups on Molecular Photoswitching of Functionalized Hemithioindigo Derivatives: a Computational Multireference Study. ChemPhotoChem, 2022, 6, .	1.5	4
12579	Slow hole transfer kinetics lead to high blend photoluminescence of unfused A ² E ² A type acceptors with unfavorable HOMO offset. Solar Rrl, 0, , .	3.1	0
12580	Best practices for first-principles simulations of epitaxial inorganic interfaces. Journal of Physics Condensed Matter, 2022, 34, 233002.	0.7	6
12581	A Mixed-Ligand Strategy to Modulate P3HT Regioregularity for High-Efficiency Solar Cells. Macromolecules, 2022, 55, 3078-3086.	2.2	26

#	ARTICLE	IF	CITATIONS
12582	Machine-learning enabled thermodynamic model for the design of new rare-earth compounds. <i>Acta Materialia</i> , 2022, 229, 117759.	3.8	13
12583	Potential forensic markers from synthetic pathways to 1-phenyl-2-propanone from uncontrolled and controlled substances. <i>Forensic Chemistry</i> , 2022, 28, 100410.	1.7	4
12584	DFT, MD simulations and experimental analysis of adsorptive complexation and isotope separation of gadolinium ion with macrocyclic crown ether embedded polymeric resin. <i>Separation and Purification Technology</i> , 2022, 289, 120709.	3.9	8
12585	Activation of carbon-hydrogen bonds by complexes involving multiply bonded Group 13 elements. <i>Polyhedron</i> , 2022, 219, 115797.	1.0	1
12586	Role of d-orbital electrons in tuning multifunctional spintronic action in pi-stacked C _n -C ₆ H ₆ -Fe-C ₆ H ₆ -C ₁₃ -n. <i>Chemical Physics</i> , 2022, 558, 111507.	0.9	0
12587	Synthesis, DFT computations, molecular docking studies and anticancer activity of 2-(4-fluorophenyl)-3-(5-methylisoxazol-3-yl)thiazolidin-4-one. <i>Chemical Data Collections</i> , 2022, 39, 100859.	1.1	5
12588	DFT studies of protonation and anion binding of Chatt type dinitrogen complex: Who is first?. <i>Inorganica Chimica Acta</i> , 2022, 536, 120899.	1.2	1
12589	Push-pull dyes based on Michler's aldehyde: Design and characterization of the optical and electrochemical properties. <i>Dyes and Pigments</i> , 2022, 202, 110278.	2.0	4
12590	Selective extraction of lithium from seawater desalination concentrates: Study of thermodynamic and equilibrium properties using Density Functional Theory (DFT). <i>Desalination</i> , 2022, 532, 115704.	4.0	14
12591	First-principles study of the effects of native defects on the thermoelectric properties of narrow-gap semiconducting δ -SrSi ₂ using the hybrid functional method. <i>Physica B: Condensed Matter</i> , 2022, 634, 413795.	1.3	0
12592	The His23 and Lys79 pair determines the high catalytic efficiency of the inorganic pyrophosphatase of the haloacid dehalogenase superfamily. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2022, 1866, 130128.	1.1	1
12593	DFT, DFTB and TD-DFT theoretical investigations of π -conjugated molecules based on thieno[2,3-b]indole for dye-sensitized solar cell applications. <i>Physica B: Condensed Matter</i> , 2022, 636, 413850.	1.3	16
12594	Electronic structure, optical properties, and electron dynamics in organic dye-sensitized TiO ₂ interfaces by local hybrid density functionals. <i>Chemical Physics</i> , 2022, 559, 111521.	0.9	2
12595	Adsorption of Ru ₂ O ₄ on Fe, Ni, Co, and Cu-doped MoS ₂ monolayer and effect of applied electric field: A DFT study. <i>Chemical Physics Letters</i> , 2022, 798, 139611.	1.2	3
12596	An account of chronological computational investigations to ascertain the role of π - π bonding in influencing the Lewis acidity of BX ₃ (X = F, Cl, Br and I): Evolution of novel parameters and relegation of π -type back bonding concept. <i>Coordination Chemistry Reviews</i> , 2022, 463, 214519.	9.5	3
12597	Novel meso-substituted dipyrromethanes based on ethyl 1,2-dimethyl-1H-pyrrole-3-carboxylate: Synthesis, X-ray and DFT study. <i>Journal of Molecular Structure</i> , 2022, 1260, 132752.	1.8	0
12598	Spectral characterization of the main pigments in the plant photosynthetic apparatus by theory and experiment. <i>Chemical Physics</i> , 2022, 559, 111517.	0.9	9
12599	Determination of dissolved nickel in natural waters using a rapid microplate fluorescence assay method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 275, 121170.	2.0	2

#	ARTICLE	IF	CITATIONS
12600	Spectroscopic and theoretical studies of some 2-(2-ethylsulfanyl)acetyl-5-substituted furans and thiophenes. <i>Journal of Molecular Structure</i> , 2022, 1261, 132895.	1.8	1
12601	Experimental and DFT studies of a novel Schiff base sulfonamide derivative ligand and its palladium (II) and platinum (IV) complexes: antimicrobial activity, cytotoxicity, and molecular docking study. <i>Journal of Molecular Structure</i> , 2022, 1261, 132811.	1.8	13
12602	Synthesis, crystal structure, DFT studies and Hirshfeld surface analysis of Manganese(II) and Cadmium(II) coordination polymers of 2-aminopyridine and dicyanamide. <i>Journal of Molecular Structure</i> , 2022, 1261, 132956.	1.8	8
12603	Benchmark Study of Computational Methods for Predicting Partition Coefficient of Chlormethiazole. <i>El-Cezeri Journal of Science and Engineering</i> , 0, , .	0.1	0
12604	Quantum Chemical Insight into Molecular Structure, Spectroscopic and Nonlinear Optical Studies on Methylene bis(dithiobenzoate). <i>Optics and Spectroscopy (English Translation of Optika I) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 10 577 Td (</i>		
12605	Crystal Structure and Energetics of Arsenic(III)-Oxide Intercalates with Rubidium Chloride and Their Comparison with Isostructural Intercalates of Potassium Halides. <i>Crystal Growth and Design</i> , 2022, 22, 711-717.	1.4	2
12606	Quantum Chemical Calculations on Fentanyl Used as Potent Analgesic. <i>NATURENGS MTU Journal of Engineering and Natural Sciences Malatya Turgut Ozal University</i> , 0, , .	0.2	0
12607	Multicomponent heat-bath configuration interaction with the perturbative correction for the calculation of protonic excited states. <i>Journal of Chemical Physics</i> , 2021, 155, 234107.	1.2	4
12608	Charge transfer excitations and constrained density functional theory. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1.	0.5	8
12609	The GW Miracle in Many-Body Perturbation Theory for the Ionization Potential of Molecules. <i>Frontiers in Chemistry</i> , 2021, 9, 749779.	1.8	32
12610	Electronic Energy and Local Property Errors at QAIM Critical Points while Climbing Perdew's Ladder of Density-Functional Approximations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 293-308.	2.3	14
12611	Structure assignment, conformational properties and discovery of potential targets of the Ugi cinnamic adduct NGI25. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-14.	2.0	3
12612	Density Functional Theory Studies of Some Barbiturates on Lipophilicity. <i>Adıyaman University Journal of Science</i> , 0, , .	0.0	0
12613	Electronic Structure of (Organic)Inorganic Metal Halide Perovskites: The Dilemma of Choosing the Right Functional. <i>Advanced Theory and Simulations</i> , 2022, 5, .	1.3	9
12614	Plasmonic 2D Materials: Overview, Advancements, Future Prospects and Functional Applications. , 0, , .		4
12615	Corrosion Resistance of Ultrathin Two-Dimensional Coatings: First-Principles Calculations towards In-Depth Mechanism Understanding and Precise Material Design. <i>Metals</i> , 2021, 11, 2011.	1.0	4
12616	Rational Design of Highly Soluble and Crystalline Conjugated Polymers for High-Performance Field-Effect Transistors. <i>Advanced Electronic Materials</i> , 2022, 8, .	2.6	10
12617	Experimentally and theoretically via high quality density function theory modelling technique and nonlinear optical analyses of 2,6-Dimethoxy-4-hydroxybenzaldehyde. <i>Materials Today: Proceedings</i> , 2022, 59, 636-641.	0.9	4

#	ARTICLE	IF	CITATIONS
12618	HSEH1PBE/6-31G(d,p) Methods Applied to Molecular Geometry and Electronic properties of Cs-C60 Cl6 Molecule. Adıyaman University Journal of Science, 0, , .	0.0	0
12619	STRUCTURAL ASPECTS OF trans-cis ISOMERIZATION OF AZOBENZENE, 4,4'-AZOPYRIDINE, AND AZOXYBENZENE. Journal of Structural Chemistry, 2021, 62, 1976-1987.	0.3	3
12620	Computational Study of Catalytic Urethane Formation. Polymers, 2022, 14, 8.	2.0	7
12621	Reaction Path Determination of Rhodium(I)-Catalyzed C-H Alkylation of N-8-Aminoquinoliny Aromatic Amides with Maleimides. Journal of Organic Chemistry, 2022, 87, 737-743.	1.7	5
12622	Metal-Metal-to-Ligand Charge Transfer in Pt(II) Dimers Bridged by Pyridyl and Quinoline Thiols. Inorganic Chemistry, 2022, 61, 121-130.	1.9	16
12623	Iridium(VII)-Corrole Terminal Carbides Should Exist as Stable Compounds. ACS Organic & Inorganic Au, 2022, 2, 159-163.	1.9	4
12624	Benchmarking the Accuracy of the Direct Random Phase Approximation and ĩf-Functionals for NMR Shieldings. Journal of Chemical Theory and Computation, 2022, 18, 192-205.	2.3	3
12625	Exploring the reaction pathway involved in the dibenzo-18-crown-6 synthesis from catechol and bis(2-chloroethyl) ether in presence of base. Journal of Physical Organic Chemistry, 2022, 35, .	0.9	1
12626	Theoretical Study of CO Adsorption Interactions with Cr-Doped Tungsten Oxide/Graphene Composites for Gas Sensor Application. ACS Omega, 2022, 7, 528-539.	1.6	8
12627	Flexible boundary layer using exchange for embedding theories. II. QM/MM dynamics of the hydrated electron. Journal of Chemical Physics, 2021, 155, 224113.	1.2	11
12628	Piecewise Multipole-Expansion Implicit Solvation for Arbitrarily Shaped Molecular Solutes. Journal of Chemical Theory and Computation, 2022, 18, 461-478.	2.3	2
12629	Theoretical Modeling of Exo- and Endohedral Hydrogenation Reactions of the Doped Magnesium Cluster Mg17Ni. Russian Journal of Inorganic Chemistry, 2021, 66, 1860-1867.	0.3	4
12630	Extraction of a One-Particle Reduced Density Matrix from a Quantum Monte Carlo Electronic Density: A New Tool for Studying Nondynamic Correlation. Computation, 2021, 9, 135.	1.0	1
12631	Low-Rank Approximations Accelerated Plane-Wave Hybrid Functional Calculations with k-Point Sampling. Journal of Chemical Theory and Computation, 2022, 18, 206-218.	2.3	17
12632	Protonation of Serine in Gas and Condensed and Microsolvated States in Aqueous Solution. Journal of Physical Chemistry A, 2022, 126, 44-52.	1.1	0
12633	Boosting O ₂ Reduction and H ₂ O Dehydrogenation Kinetics: Surface N-Hydroxymethylation of g-C ₃ N ₄ Photocatalysts for the Efficient Production of H ₂ O ₂ . Advanced Functional Materials, 2022, 32, .	7.8	76
12634	BH9, a New Comprehensive Benchmark Data Set for Barrier Heights and Reaction Energies: Assessment of Density Functional Approximations and Basis Set Incompleteness Potentials. Journal of Chemical Theory and Computation, 2022, 18, 151-166.	2.3	27
12635	Systematic Evaluation of Modern Density Functional Methods for the Computation of NMR Shifts of 3d Transition-Metal Nuclei. Journal of Chemical Theory and Computation, 2022, 18, 273-292.	2.3	11

#	ARTICLE	IF	CITATIONS
12636	Theoretical unraveling of the separation of trivalent Am and Eu ions by phosphine oxide ligands with different central heterocyclic moieties. Dalton Transactions, 2022, 51, 7118-7126.	1.6	10
12637	A unique electronic state in a ferromagnetic semiconductor FeCl ₂ monolayer. Journal of Materials Chemistry C, 2022, 10, 8009-8014.	2.7	8
12638	Realizing high-rate aqueous zinc-ion batteries using organic cathode materials containing electron-withdrawing groups. Sustainable Energy and Fuels, 2022, 6, 2523-2531.	2.5	21
12639	Molecular structure determination, spectroscopic, quantum computational studies and molecular Structure and Dynamics, 2023, 41, 3574-3590.	2.0	9
12640	Assessing the effect of a series of mutations on the dynamic behavior of phosphite dehydrogenase using molecular docking, molecular dynamics and quantum mechanics/molecular mechanics simulations. Journal of Biomolecular Structure and Dynamics, 2023, 41, 4154-4166.	2.0	7
12641	Relativistic Orbital-Optimized Density Functional Theory for Accurate Core-Level Spectroscopy. Journal of Physical Chemistry Letters, 2022, 13, 3438-3449.	2.1	24
12642	Chiral photochemistry of achiral molecules. Nature Communications, 2022, 13, 2091.	5.8	11
12643	Synthesis, structural characterization, antioxidant and antidiabetic activities, DFT calculation, and molecular docking of novel substituted phenolic and heterocyclic compounds. Journal of Biomolecular Structure and Dynamics, 2022, , 1-13.	2.0	0
12644	How Ionization Catalyzes Diels-Alder Reactions. Chemistry - A European Journal, 2022, 28, .	1.7	5
12645	The Lanthanide Contraction Is a Variable. Inorganic Chemistry, 2022, 61, 6120-6127.	1.9	6
12646	Assessing Alkene Reactivity toward Cytochrome P450-Mediated Epoxidation through Localized Descriptors and Regression Modeling. Journal of Chemical Information and Modeling, 2022, 62, 1979-1987.	2.5	4
12647	Lewis acid stabilized group 13-15 element analogs of ethylene. Journal of Computational Chemistry, 2023, 44, 218-228.	1.5	3
12648	Molecular Principles of Redox-Coupled Protonation Dynamics in Photosystem II. Journal of the American Chemical Society, 2022, 144, 7171-7180.	6.6	35
12649	Study on Zr, Sn, Pb, Si and Pt doped TiO ₂ photoanode for dye-sensitized solar cells: The first-principles calculations. Chemical Physics Letters, 2022, 799, 139636.	1.2	4
12650	Structures, Energetics, and Spectra of (NH) and (OH) Tautomers of 2-(2-Hydroxyphenyl)-1-azaazulene: A Density Functional Theory/Time-Dependent Density Functional Theory Study. ACS Omega, 2022, 7, 14222-14238.	1.6	4
12651	Structural, vibrational and thermodynamic properties of the isomers of the dimer molecules Ba ₂ X ₄ (X = F, Cl, Br, or I). Structural Chemistry, 2022, 33, 1285-1294.	1.0	1
12652	Roles of Ligand and Oxidant in Pd(II)-Catalyzed and Ligand-Enabled C(sp ³)-H Lactonization in Aliphatic Carboxylic Acid: Mechanistic Studies. ACS Catalysis, 2022, 12, 4848-4858.	5.5	11
12653	PTB7-Th-Based Organic Photovoltaic Cells with a High <i>V</i> _{OC} of over 1.0 V <i>via</i> Fluorination and Side Chain Engineering of Benzotriazole-Containing Nonfullerene Acceptors. ACS Applied Materials & Interfaces, 2022, 14, 18764-18772.	4.0	15

#	ARTICLE	IF	CITATIONS
12654	Conformational Properties of New Thiosemicarbazone and Thiocarbohydrazone Derivatives and Their Possible Targets. <i>Molecules</i> , 2022, 27, 2537.	1.7	8
12655	Review on the QM/MM Methodologies and Their Application to Metalloproteins. <i>Molecules</i> , 2022, 27, 2660.	1.7	28
12656	Exploring Detailed Reaction Pathways for Hydrogen Storage with Borohydrides Using DFT Calculations. <i>Energy & Fuels</i> , 2022, 36, 5513-5527.	2.5	2
12657	Noncanonical Isomers of Nucleoside Cation Radicals: An Ab Initio Study of the Dark Matter of DNA Ionization. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2480-2497.	1.1	4
12658	Double Hybrids and Noncovalent Interactions: How Far Can We Go?. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2590-2599.	1.1	9
12659	Examining the Role of Aryldiazonium Salts in Surface Electroinitiated Polymerization. <i>Langmuir</i> , 2022, 38, 4979-4995.	1.6	5
12660	Tracing the Primordial Chemical Life of Glycine: A Review from Quantum Chemical Simulations. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4252.	1.8	12
12661	Si-containing 3D cage-functionalized graphene oxide grafted with Ferrocene for high-performance supercapacitor application: An experimental and theoretical study. <i>Journal of Energy Storage</i> , 2022, 50, 104635.	3.9	9
12662	Simple development of eco-friendly dye-sensitized solar cells via controlling thickness of TiO ₂ nanoparticles and viscosity of electrolyte: Experimental study and DFT calculations. <i>Inorganic Chemistry Communication</i> , 2022, 140, 109472.	1.8	1
12678	Stereochemical dependence of substituent ¹³ C effects in the ¹⁹ F NMR shielding constants. <i>Magnetic Resonance in Chemistry</i> , 2022, 60, 869-876.	1.1	1
12679	Towards an atomistic understanding of polymorphism in molecular solids. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11278-11294.	1.3	4
12680	Combustion Kinetics of N-Propylamine: Theoretical Calculations and Ignition Delay Time Measurements. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12681	Computational studies on the possible formation of glycine <i>via</i> open shell gas-phase chemistry in the interstellar medium. <i>Organic and Biomolecular Chemistry</i> , 2022, , .	1.5	2
12682	Understanding the internal heavy-atom effect on thermally activated delayed fluorescence: application of Arrhenius and Marcus theories for spin-orbit coupling analysis. <i>Journal of Materials Chemistry C</i> , 2022, 10, 7925-7934.	2.7	18
12683	Electronic structure and magnetic coupling in selenium substituted pyridine-bridged bisdithiazolyl multifunctional molecular materials. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12196-12207.	1.3	2
12684	Noncovalently bound excited-state dimers: a perspective on current time-dependent density functional theory approaches applied to aromatic excimer models. <i>RSC Advances</i> , 2022, 12, 13014-13034.	1.7	18
12685	TAO-DFT fictitious temperature made simple. <i>RSC Advances</i> , 2022, 12, 12193-12210.	1.7	7
12686	Identification of new pyrazolyl piperidine molecules as factor Xa inhibitors: Design, synthesis, in silico, and biological evaluation. <i>Results in Chemistry</i> , 2022, 4, 100355.	0.9	4

#	ARTICLE	IF	CITATIONS
12687	Turn on Fluorescence Sensing of Zn ²⁺ Based on Fused Isoindole-Imidazole Scaffold. <i>Molecules</i> , 2022, 27, 2859.	1.7	9
12688	New magnetic-fluorescent bifunctional (Y _{0.9} Ln _{0.1} VO ₄ /Fe ₃ O ₄)@SiO ₂ and [(Y _{0.9} Ln _{0.1} VO ₄ @SiO ₂)/Fe ₃ O ₄ @SiO ₂] materials. <i>Ceramics International</i> , 2022, 48, 22006-22017.	2.3	4
12689	Titration of Cu(I) Sites in Cu-ZSM-5 by Volumetric CO Adsorption. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 21059-21068.	4.0	12
12690	Binding and Degradation Reaction of Hydroxide Ions with Several Quaternary Ammonium Head Groups of Anion Exchange Membranes Investigated by the DFT Method. <i>Molecules</i> , 2022, 27, 2686.	1.7	12
12691	Computer-Aided Design of Fluorinated Flavin Derivatives by Modulation of Intersystem Crossing and Fluorescence. <i>ChemPhotoChem</i> , 2022, 6, .	1.5	5
12692	Cationic Axial Ligand Effects on Sulfur-Substituted Subphthalocyanines. <i>Molecules</i> , 2022, 27, 2766.	1.7	2
12693	Kalihioxepanes <sc>A</sc> : Seven Kalihinene Diterpenoids from Marine Sponge <i>Acanthella cavernosa</i> Collected off the South China Sea. <i>Chinese Journal of Chemistry</i> , 0, , .	2.6	6
12694	Raman Fingerprints of π -Electron Delocalization in Polythiophene-Based Insulated Molecular Wires. <i>Macromolecules</i> , 2022, 55, 3458-3468.	2.2	10
12695	Unlocking New Redox Activity in Alluaudite Cathodes through Compositional Design. <i>Chemistry of Materials</i> , 2022, 34, 4088-4103.	3.2	5
12696	Cyclodextrin-Activated Porphyrin Photosensitization for Boosting Self-Cleavable Drug Release. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 6764-6774.	2.9	12
12697	Insights into the insertion reaction mechanism of phosphonium cation and oxirane: a theoretical study. <i>Journal of Chemical Sciences</i> , 2022, 134, .	0.7	0
12698	A theoretical investigation of nonlinear optical and electronic molecular parameters of hexabutyloxytryphenylene and halogenated hexabutyloxytryphenylene molecules using density functional theory (DFT) for nonlinear device applications. <i>Physica Scripta</i> , 2022, 97, 065808.	1.2	7
12699	Conformational preferences and intramolecular hydrogen bonding patterns of tetraflavaspidic acid BBBB " a tetrameric acylphloroglucinol. <i>ChemistrySelect</i> , 2022, .	0.7	0
12700	The effect of intramolecular and intermolecular charge transfers on the third order nonlinear optical properties of the self-assemble chromophores. <i>Journal of Luminescence</i> , 2022, , 118991.	1.5	1
12701	Modulation of Intersystem Crossing by Chemical Composition and Solvent Effects: Benzophenone, Anthrone and Fluorenone. <i>ChemPhotoChem</i> , 2022, 6, .	1.5	4
12702	<sc>Gas</sc>Phase Ion<sc>Molecule</sc> Interactions in a Collision Reaction Cell with <sc>ICP</sc><sc>MS</sc>: Investigations with <sc>CO₂</sc> as the Reaction Gas. <i>Geostandards and Geoanalytical Research</i> , 2022, 46, 387-399.	1.7	6
12703	Optoelectronic features of NbCu ₃ Q ₄ (Q = S, Se) for p-type transparent conducting application: DFT and HSE06. <i>Optik</i> , 2022, 262, 169297.	1.4	3
12704	Assessment of XC functionals for the study of organic molecules with superhalogen substitution. A systematic comparison between DFT and CCSD(T). <i>Journal of Chemical Physics</i> , 2022, 156, 184303.	1.2	4

#	ARTICLE	IF	CITATIONS
12705	HCnH ⁿ Anion Chains with n ≥ 8 Are Nonlinear and Their Permanent Dipole Makes Them Potential Candidates for Astronomical Observation. <i>Molecules</i> , 2022, 27, 3100.	1.7	7
12706	Comparative Study of Vibrational Raman Optical Activity with Different Time-Dependent Density Functional Approximations: The VROA36 Database. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2909-2927.	1.1	4
12707	Harnessing Colossal Magnetic Anisotropy in Sandwiched 3d ² -Metalloenes. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2811-2817.	1.1	5
12708	A Closed Local-Orbital Unified Description of DFT and many-body effects. <i>Journal of Physics Condensed Matter</i> , 2022, , .	0.7	1
12709	Rate constant and mechanism of the OH-initiated degradation of 3-penten-2-one in the atmosphere. <i>Computational and Theoretical Chemistry</i> , 2022, 1213, 113737.	1.1	0
12710	Predicting the modulation of UV-vis absorption and emission of mono-substituted pyrido[2,3,4-kl]acridines by electronic density variations analysis. <i>Computational and Theoretical Chemistry</i> , 2022, 1213, 113733.	1.1	0
12711	Theoretical investigation of the electronic structure of the ground and lowest excited states with dipole moment and rovibrational calculations of the CuSe molecule. <i>Chemical Physics Letters</i> , 2022, 800, 139653.	1.2	0
12712	Investigation of W/Mo co-doping with multiple concentrations in photocatalyst BiVO ₄ by first-principles calculations. <i>Solid State Communications</i> , 2022, 351, 114794.	0.9	2
12713	Efficient separation of strontium ions from aqueous solution by dibenzo-18-crown-6 functionalized resin: Static and dynamic adsorption studies with computational DFT insights. <i>Chemical Engineering Journal Advances</i> , 2022, 11, 100308.	2.4	7
12714	Fluorescent Cu ²⁺ sensor based on phenanthroline-BODIPY conjugate: A mechanistic study. <i>Dyes and Pigments</i> , 2022, 203, 110343.	2.0	12
12715	Optoelectronic and vibrational properties of chalcogenides VCu ₃ Q ₄ (Q= Se, Te) for potential p-type transparent conducting materials: HSE06 approach. <i>Journal of Solid State Chemistry</i> , 2022, 312, 123190.	1.4	4
12716	Bidentate ligand modification strategy on supported Ni nanoparticles for photocatalytic selective hydrogenation of alkynes. <i>Applied Catalysis B: Environmental</i> , 2022, 313, 121449.	10.8	8
12717	Synthesis, experimental and theoretical analyses of bis(2-ethylphenyl)phosphorodithioates of nickel(II). <i>Journal of Molecular Structure</i> , 2022, 1263, 133166.	1.8	3
12718	Theoretical investigation of electronic structures, second-order NLO responses of cyclometalated Ir(III) and Rh(III) counterpart complexes: effect of metal centers. <i>New Journal of Chemistry</i> , 2022, 46, 10652-10661.	1.4	7
12719	Modification of benzoindenthioephene-based organic dye with fused thiophenes for efficient dye-sensitized solar cells. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 115, 108214.	1.3	1
12720	New insights on nonlinear solvatochromism in binary mixture of solvents. <i>Advances in Quantum Chemistry</i> , 2022, , .	0.4	0
12722	Recommendation of Orbitals for GW Calculations on Molecules and Crystals. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3523-3537.	2.3	3
12723	DFT Rationalization of Gold(I)-Catalyzed Couplings between Alkynyl Thioether and Nitrenoid Derivatives: Mechanism, Selectivity Patterns, and Effects of Substituents. <i>Journal of Organic Chemistry</i> , 2022, 87, 7193-7201.	1.7	4

#	ARTICLE	IF	CITATIONS
12724	Assessing Recent Time-Dependent Double-Hybrid Density Functionals on Doublet–Doublet Excitations. ACS Physical Chemistry Au, 2022, 2, 407-416.	1.9	3
12725	Machine Learning Screening of Efficient Ionic Liquids for Targeted Cleavage of the β -O-4 Bond of Lignin. Journal of Physical Chemistry B, 2022, 126, 3693-3704.	1.2	6
12726	Enhanced photocatalysis and photodetection using highly crystalline CZTS thin films optimized using stabilizers. Ceramics International, 2022, 48, 35666-35675.	2.3	9
12727	Ultra-Long Lived Luminescent Triplet Excited States in Cyclic (Alkyl)(amino)carbene Complexes of Zn(II) Halides. Chemistry - A European Journal, 2022, 28, .	1.7	15
12728	One-dimensional magnetism in a facile spin 1/2 Heisenberg antiferromagnet with a low saturation field. CrystEngComm, 2022, 24, 4910-4920.	1.3	1
12729	Copper(II) and zinc(II) complexation with <i>N</i> -ethylene hydroxycyclams and consequences on the macrocyclic backbone configuration. Dalton Transactions, 0, , .	1.6	5
12730	An experimental and theoretical charge density study of theophylline and malonic acid cocrystallization. RSC Advances, 2022, 12, 15670-15684.	1.7	5
12731	Vibronic effects accelerate the intersystem crossing processes of the through-space charge transfer states in the triptycene bridged acridine–triazine donor–acceptor molecule TpAT-tFFO. Chemical Science, 2022, 13, 7057-7066.	3.7	9
12732	Machine learning accelerated search for new double perovskite oxide photocatalysis. Wuli Xuebao/Acta Physica Sinica, 2022, 71, 177101.	0.2	2
12733	Mechanistic Studies on Nickel-Catalyzed Ethylene Polymerization: Ligand Effects and Quantitative Structure–Activity Relationship Model. Organometallics, 2022, 41, 3212-3218.	1.1	3
12734	Unraveling the effect of sulfur doping into electronic and optical performance of monoclinic hafnium dioxide (m-HfO ₂ : S): an (DFT+U) insights report. Applied Physics A: Materials Science and Processing, 2022, 128, .	1.1	3
12735	Open-Form Configurational Isomers of a Tricyanofuran-Type Metastable-State Photoacid. ACS Omega, 0, , .	1.6	0
12736	SERS-Based Ultralow Concentration Detection of Anticancer Gemcitabine Using Size-Controlled Silver Nanoparticles. Arabian Journal for Science and Engineering, 2022, 47, 7197-7205.	1.7	2
12737	In Situ Observation of the Structure of Crystallizing Magnesium Sulfate Heptahydrate Solutions with Terahertz Transmission Spectroscopy. Crystal Growth and Design, 0, , .	1.4	1
12738	Insight of development of two cured epoxy polymer composite coatings as highly protective efficiency for carbon steel in sodium chloride solution: DFT, RDF, FFV and MD approaches. Journal of Molecular Liquids, 2022, 360, 119406.	2.3	35
12739	Comparative QM/MM study on the inhibition mechanism of β -Hydroxynorvaline to Threonyl-tRNA synthetase. Journal of Molecular Graphics and Modelling, 2022, 115, 108224.	1.3	4
12740	Computational and experimental study of different brines in temperature swing solvent extraction desalination with amine solvents. Desalination, 2022, 537, 115863.	4.0	12
12741	Computational investigation of substituent effects on the fluorescence wavelengths of oxyluciferin analogs. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 431, 114018.	2.0	1

#	ARTICLE	IF	CITATIONS
12742	Contact Analysis of Elemental Transition Metal Electrodes for Complementary 2D-FET Applications Using MoS ₂ and WSe ₂ . IEEE Electron Device Letters, 2022, 43, 1137-1140.	2.2	0
12743	Multinuclear Ni(II) and Cu(II) complexes of a meso-6 + 6 macrocyclic amine derived from trans-1,2-diaminocyclopentane and 2,6-diformylpyridine. Dalton Transactions, 2022, 51, 9735-9747.	1.6	10
12744	Proton-Transfer Reactions of Re(I)-Nitrosyl Complexes: Potentiometric Studies, Dft and Td-Dft Calculations. SSRN Electronic Journal, 0, , .	0.4	0
12745	Mechanistic and Kinetic Insights into the Atmospheric Degradation of (CH ₃) ₃ CF and (CH ₃) ₃ CCl Initiated by Cl Atom. SSRN Electronic Journal, 0, , .	0.4	0
12746	Improved Photovoltaic Performances of Coumarin Derivatives by Forming D-A ² -A Structure Using Diketopyrrolopyrrole as Auxiliary Acceptor. SSRN Electronic Journal, 0, , .	0.4	1
12747	Processing and interpretation of core-electron XPS spectra of complex plasma-treated polyethylene-based surfaces using a theoretical peak model. Surface and Interface Analysis, 0, , .	0.8	0
12748	SimStack: An Intuitive Workflow Framework. Frontiers in Materials, 2022, 9, .	1.2	5
12749	In Silico Optimization of Charge Separating Dyes for Solar Energy Conversion. ChemSusChem, 0, , .	3.6	3
12750	A mechanistic view of the reaction between phosphine and fluorine atom: Insights into PH ₃ F isomers. Computational and Theoretical Chemistry, 2022, 1214, 113769.	1.1	0
12751	4-Amino-1-butyl-1,2,4-triazolium Dinitramide – Synthesis, Characterization and Combustion of a Low-Temperature Dinitramide-Based Energetic Ionic Liquid (EIL). Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.0	5
12752	Mechanistic Insights into Enzyme Catalysis from Explaining Machine-Learned Quantum Mechanical and Molecular Mechanical Minimum Energy Pathways. ACS Physical Chemistry Au, 2022, 2, 316-330.	1.9	5
12753	Conversion of Sewage Water into H ₂ Gas Fuel Using Hexagonal Nanosheets of the Polyaniline-Assisted Deposition of PbI ₂ as a Nanocomposite Photocathode with the Theoretical Qualitative Ab-Initio Calculation of the H ₂ O Splitting. Polymers, 2022, 14, 2148.	2.0	8
12754	A ROS-Responsive Simvastatin Nano-Prodrug and its Fibronectin-Targeted Co-Delivery System for Atherosclerosis Treatment. ACS Applied Materials & Interfaces, 2022, 14, 25080-25092.	4.0	11
12755	Ab Initio Calculation of Surface-Controlled Photocatalysis in Multiple-Phase BiVO ₄ . Journal of Physical Chemistry C, 2022, 126, 9541-9550.	1.5	6
12756	Regression Modeling for the Prediction of Hydrogen Atom Transfer Barriers in Cytochrome P450 from Semi-empirically Derived Descriptors. Chemistry Methods, 2022, 2, .	1.8	2
12757	Bromoacetic Acid-Promoted Nonheme Manganese-Catalyzed Alkane Hydroxylation Inspired by β -Ketoglutarate-Dependent Oxygenases. ACS Catalysis, 2022, 12, 6756-6769.	5.5	17
12758	Top-down formation of ethylene from fragmentation of superhydrogenated polycyclic aromatic hydrocarbons. Astronomy and Astrophysics, 2022, 663, A150.	2.1	4
12759	Computational study of 2N-atom functionalized corannulene by alkali metals doping: Towards the development of highly efficient nonlinear optical materials. Physica B: Condensed Matter, 2022, 640, 414041.	1.3	14

#	ARTICLE	IF	CITATIONS
12760	Reactivity of 4,5-Dichlorophthalic Anhydride towards Thiosemicarbazide and Amines: Synthesis, Spectroscopic Analysis, and DFT Study. <i>Molecules</i> , 2022, 27, 3550.	1.7	5
12761	Near-Infrared Absorbing Molecule Based on Triphenylamine Radical Cation with Extended Homoaryl π -System. <i>Colorants</i> , 2022, 1, 226-235.	0.9	3
12762	Accelerating <i>Ab Initio</i> Quantum Mechanical and Molecular Mechanical (QM/MM) Molecular Dynamics Simulations with Multiple Time Step Integration and a Recalibrated Semiempirical QM/MM Hamiltonian. <i>Journal of Physical Chemistry B</i> , 2022, 126, 4226-4235.	1.2	6
12763	The structural origin of the efficient photochromism in natural minerals. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	8
12764	Molecular Orientation-Induced Second-Harmonic Generation: Deciphering Different Contributions Apart. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3732-3738.	1.1	5
12765	Theoretical Distribution of the Ammonia Binding Energy at Interstellar Icy Grains: A New Computational Framework. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 1514-1526.	1.2	18
12766	Tetrahydropyridin-4-ylpicolinoylglycines as novel and orally active prolyl hydroxylase 2 (PHD2) inhibitors for the treatment of renal anemia. <i>European Journal of Medicinal Chemistry</i> , 2022, 238, 114479.	2.6	3
12767	Experimental and theoretical approach for novel imidazolium ionic liquids as Smart Corrosion inhibitors for mild steel in 1.0M hydrochloric acid. <i>Arabian Journal of Chemistry</i> , 2022, 15, 103967.	2.3	14
12768	Mixed-valence outer-sphere RuII/RuIII ion-pair complexes. Synthesis, experimental, and theoretical studies. <i>Polyhedron</i> , 2022, 223, 115939.	1.0	2
12769	Spectroscopic (UV-vis, FT-IR, FT-Raman, and NMR) analysis, structural benchmarking, molecular properties, and the in-silico cerebral anti-ischemic activity of 2-amino-6-ethoxybenzothiazole. <i>Journal of Molecular Structure</i> , 2022, 1265, 133318.	1.8	28
12773	A Brief on Nuclear Waste at the Hanford Site and a Computational Analysis of Uranyl Nitrate with and without Tributyl Phosphate. <i>ACS Symposium Series</i> , 0, , 101-129.	0.5	2
12774	An Introduction to High Performance Computing and Its Intersection with Advances in Modeling Rare Earth Elements and Actinides. <i>ACS Symposium Series</i> , 0, , 3-53.	0.5	3
12775	The effect of structural configuration on the DNA binding and <i>in vitro</i> antioxidant properties of new copper(N_2O_2) Schiff base complexes. <i>New Journal of Chemistry</i> , 2022, 46, 12968-12980.	1.4	7
12776	Nitrene-Mediated Multicomponent Couplings and Macrocyclization by CH-Functionalization. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12777	Theoretical Investigation by DFT and TDDFT the Extension of π -Conjugation of Novel Carbazole-Based Donor Materials for Bulk Heterojunction Organic Solar Cell Applications. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12778	Refining details of the structural and electronic properties of the Cu_B site in pMMO enzyme through sequential molecular dynamics/CPKS-EPR calculations. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
12779	Electronic structure of strongly correlated systems: recent developments in multiconfiguration pair-density functional theory and multiconfiguration nonclassical-energy functional theory. <i>Chemical Science</i> , 2022, 13, 7685-7706.	3.7	18
12780	Structural and Photoelectrochemical Dynamics of In-Situ Hydrogenated Anatase TiO_2 Thin Films Grown by DC Reactive Magnetron Sputtering. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
12781	Theoretical study on the mechanism, chemo- and enantioselectivity of the Ag- vs. Rh-catalyzed intramolecular carbene transfer reaction of diazoacetamides. <i>RSC Advances</i> , 2022, 12, 18197-18208.	1.7	1
12782	Effect of Substituent on C-H Activation Catalysed by a nonheme Fe(IV)O Complex: A Computational Investigation of Reactivity and Hydrogen Tunneling. <i>Dalton Transactions</i> , 0, , .	1.6	1
12783	Non-covalent interactions atlas benchmark data sets 4: π -hole interactions. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14794-14804.	1.3	27
12784	Computational descriptor analysis on excited state behaviours of a series of TADF and non-TADF compounds. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16167-16182.	1.3	6
12785	A transferable prediction model of molecular adsorption on metals based on adsorbate and substrate properties. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16545-16555.	1.3	3
12786	Modeling of the Electrical Properties of Self-Assembled Island-Type Films of Polar C60F18 Molecules on Chemically Inactive Surfaces. <i>Journal of Surface Investigation</i> , 2022, 16, 233-246.	0.1	0
12787	Cyclization Reaction of 3,5-Diacetyl-2,6-dimethylpyridine with Salicylic Aldehyde and Its Derivatives: Quantum-Chemical Study and Molecular Docking. <i>Russian Journal of General Chemistry</i> , 2022, 92, 914-924.	0.3	2
12788	Dielectric-dependent hybrid functional calculations on the electronic band gap of Mn_3SnS_2 transition metal doped Mn_3SnS_2 and their optical properties. <i>Physical Review B</i> , 2022, 105, .	1.1	5
12789	Recovery of lithium from salt lake brine with high Na/Li ratio using solvent extraction. <i>Journal of Molecular Liquids</i> , 2022, 362, 119667.	2.3	18
12790	Stability enhancement of iron-based perovskite catalysts by Br -site substitution for oxidative transposition of Br -bromostyrene to phenacyl bromide. <i>ChemCatChem</i> , 0, , .	1.8	2
12791	Excited state non-adiabatic dynamics of large photoswitchable molecules using a chemically transferable machine learning potential. <i>Nature Communications</i> , 2022, 13, .	5.8	31
12792	Gas-Phase Peroxyl Radical Recombination Reactions: Computational Study of Formation and Decomposition of Tetroxides. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4046-4056.	1.1	9
12793	Systematically Improvable Generalization of Self-Interaction Corrected Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5698-5702.	2.1	5
12794	Insight into the Fergusonite-Scheelite Phase Transition of ABO_4 -Type Oxides by Density Functional Theory: A Case Study of the Subtleties of the Ground State of BiVO_4 . <i>Chemistry of Materials</i> , 2022, 34, 5334-5343.	3.2	6
12795	Nonlinear optical properties and optimization strategies of D-A type phenylamine derivatives in the near-infrared region. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 280, 121539.	2.0	6
12796	Excited-State Deactivation Mechanism of 3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazole: Electronic Structure Calculations and Nonadiabatic Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4002-4012.	1.1	5
12797	Source of Rate Acceleration for Carbocation Cyclization in Biomimetic Supramolecular Cages. <i>Journal of the American Chemical Society</i> , 2022, 144, 11413-11424.	6.6	15
12798	Theoretical Study of Alkaline-Earth Metal (Be, Mg, and Ca)-Substituted Aluminum Nitride Nanocages With High Stability and Large Nonlinear Optical Responses. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	0

#	ARTICLE	IF	CITATIONS
12799	Virtual Experiments on Real Asphaltenes: Predicting Properties Using Quantum Chemical Simulations of Structures from Non-contact Atomic Force Microscopy. <i>Energy & Fuels</i> , 2022, 36, 8714-8724.	2.5	6
12800	Calculating bond dissociation energies of X-H (X=C, N, O, S) bonds of aromatic systems via density functional theory: a detailed comparison of methods. <i>Royal Society Open Science</i> , 2022, 9, .	1.1	7
12802	Graph-learning guided mechanistic insights into imipenem hydrolysis in GES carbapenemases. <i>Electronic Structure</i> , 2022, 4, 034001.	1.0	2
12803	Electrodeposition and Characterization of Conducting Polymer Films Obtained from Carbazole and 2-(9H-carbazol-9-yl)acetic Acid. <i>Electrochem</i> , 2022, 3, 322-336.	1.7	0
12804	Efficiently Computing NMR ¹ H and ¹³ C Chemical Shifts of Saccharides in Aqueous Environment. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4373-4386.	2.3	6
12805	Protonation of Phosphonocarboxylates in Aqueous Medium: An Experimental and Theoretical Investigation. <i>Journal of Chemical & Engineering Data</i> , 0, , .	1.0	2
12806	Enhanced adsorption of fluoroquinolone antibiotic on the surface of the Mg-, Ca-, Fe- and Zn-doped C60 fullerenes: DFT and TD-DFT approach. <i>Materials Today Communications</i> , 2022, 31, 103798.	0.9	10
12807	Conformational Selectivity of Merocyanine on Nanostructured Silver Films: Surface Enhanced Resonance Raman Scattering (SERRS) and Density Functional Theoretical (DFT) Study. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	3
12808	DPPC phospholipid interaction with cholesterol and melatonin: Raman spectroscopy and density functional theory study. <i>Journal of Raman Spectroscopy</i> , 0, , .	1.2	1
12809	Benzenetriimide-Based Molecular Conductor with Antiferro-to Ferromagnetic Switching Induced by Structural Change of Î-stacked Array. <i>ChemPhysChem</i> , 2022, 23, .	1.0	2
12810	On the Importance of Well-Defined Thermal Correlation Functions in Simulating Vibronic Spectra. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3947-3956.	1.1	3
12811	High CT-Fluorophore Featuring a Basic Moiety into D-A Chain as a p <i>K_a</i> Probe. <i>Journal of Organic Chemistry</i> , 2022, 87, 7618-7634.	1.7	4
12812	Unraveling the Reaction Mechanism of Mo/Cu CO Dehydrogenase Using QM/MM Calculations. <i>ACS Catalysis</i> , 2022, 12, 7336-7343.	5.5	9
12813	Band Edge Engineering of 2D Perovskite Structures through Spacer Cation Engineering for Solar Cell Applications. <i>Journal of Physical Chemistry C</i> , 2022, 126, 9937-9947.	1.5	6
12814	<i>N</i> -Acetyl Side-Chain Conformation in Saccharides: Solution Models Obtained from <i>MATMAT</i> Analysis. <i>Journal of Organic Chemistry</i> , 2022, 87, 8368-8379.	1.7	5
12815	Molecular Structures and Redox Properties of Homoleptic Aluminum(III) Complexes with Azobisphenolate (azp) Ligands. <i>Inorganics</i> , 2022, 10, 84.	1.2	0
12816	Comprehensive Quantum Chemical Characterization of the Astrochemically Relevant HC _n H Chain Family: An Attempt to Aid Astronomical Observations. <i>Advanced Theory and Simulations</i> , 2022, 5, .	1.3	8
12817	Reaction of Ta ₃ Clusters with Molecular Nitrogen: A Mechanism Investigation. <i>ACS Omega</i> , 2022, 7, 22682-22688.	1.6	3

#	ARTICLE	IF	CITATIONS
12818	Oxidation of Hypophosphorous Acid by a Ruthenium(VI) Nitrido Complex in Aqueous Acidic Solution. Evidence for a Proton-Coupled N-Atom Transfer Mechanism. <i>Inorganic Chemistry</i> , 2022, 61, 10567-10574.	1.9	0
12819	Complex Oxides for Brain-Inspired Computing: A Review. <i>Advanced Materials</i> , 2023, 35, .	11.1	17
12820	Conformationally Confined Emissive Cationic Macrocycle with Photocontrolled Organelle-Specific Translocation. <i>Advanced Science</i> , 2022, 9, .	5.6	6
12821	Effects of non-local exchange functionals in the density functional theories for the description of molecular vibrations. <i>Journal of Chemical Sciences</i> , 2022, 134, .	0.7	2
12822	Diphenoquinones Redux. <i>Journal of Organic Chemistry</i> , 2022, 87, 7673-7695.	1.7	1
12823	Regioselective [3+2] cycloaddition synthesis and theoretical calculations of new chromene-pyrazole hybrids: A DFT-based Parr Function, Fukui Function, local reactivity indexes, and MEP analysis. <i>Journal of Molecular Structure</i> , 2022, 1267, 133583.	1.8	22
12824	Concentration asymmetry and carbon enrichment in titanium carbide and silicon carbide clusters. <i>Physical Review A</i> , 2022, 105, .	1.0	2
12825	Revealing the regioselective N-acylation of 5-bromo-2-aminobenzimidazole using experiment and theoretical calculation. <i>Tetrahedron</i> , 2022, , 132905.	1.0	1
12826	Benchmark Density Functional Theory Approach for the Calculation of Bond Dissociation Energies of the M^{O}_{2} Bond: A Key Step in Water Splitting Reactions. <i>ACS Omega</i> , 2022, 7, 20800-20808.	1.6	9
12827	Solid-state performance of a meta-GGA screened hybrid density functional constructed from Pauli kinetic enhancement factor dependent semilocal exchange hole. <i>Journal of Chemical Physics</i> , 0, , .	1.2	4
12828	On the Viability of Divergent Donor Moieties in Malononitrile-Based Donor-Acceptor NLO active materials: A DFT/TDDFT Study. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	4
12829	Improved proton-transfer barriers with van der Waals density functionals: Role of repulsive non-local correlation. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	3
12830	Cost-effective dyes based on low-cost donors and Pd-free synthesis for dye-sensitized solar cells. <i>Solar Rrl</i> , 0, , .	3.1	0
12831	Crystal Prediction and Design of Tunable Light Emission in BTB-Based Metal-Organic Frameworks. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	3
12832	DFT study on the mechanism of the CO ₂ -to-CO conversion by Co-quaterpyridine complexes. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113794.	1.1	2
12833	Combustion kinetics of n-propylamine : Theoretical calculations and ignition delay time measurements. <i>Fuel</i> , 2022, 324, 124710.	3.4	3
12834	Insights into the transformation of VO ₂ ⁺ motif to VO ₃ ⁺ , V ₂ O ₃ ⁴⁺ and VO ₂ ⁺ motifs and their interconversion along with a detailed mechanistic study of their anti-cancer activity in SiHa cervical cancer cells. <i>Journal of Inorganic Biochemistry</i> , 2022, 234, 111900.	1.5	0
12835	Synthesis, physicochemical properties, theoretical and electrochemical studies of tetraglycidyl methylenedianiline. <i>Journal of Molecular Structure</i> , 2022, 1265, 133508.	1.8	20

#	ARTICLE	IF	CITATIONS
12836	Stabilities, electronic and piezoelectric properties of blue-phosphorene-phase MXs (M=Ge, Sn; X=S, Se). <i>Tj ETQq0 0 0 rgBT /Overlo</i>	3.1	2
12837	Maximally exploiting active sites on Yolk@shell nanoreactor: Nearly 100% PMS activation efficiency and outstanding performance over full pH range in Fenton-like reaction. <i>Applied Catalysis B: Environmental</i> , 2022, 316, 121594.	10.8	73
12838	Photocatalytic CO ₂ reduction by a Z-scheme mechanism in an aqueous suspension of particulate (CuGa) _{0.3} Zn _{1.4} S ₂ , BiVO ₄ and a Co complex operating dual-functionally as an electron mediator and as a cocatalyst. <i>Applied Catalysis B: Environmental</i> , 2022, 316, 121600.	10.8	8
12839	Ultrafast Förster resonance energy transfer between tyrosine and tryptophan: potential contributions to protein-water dynamics measurements. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18055-18066.	1.3	4
12840	Exploring the photophysical properties of unusual π -conjugated porphyrin nanohoops. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
12841	Dynamics of Electron Collision with Potential Biofuel: n-Butanol. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12842	Magnetic couplings and applied electric field regulation in diradical SiC defect diamond-like nanoclusters. <i>New Journal of Chemistry</i> , 2022, 46, 14676-14689.	1.4	1
12843	Exploration of the photocatalytic cycle for sacrificial hydrogen evolution by conjugated polymers containing heteroatoms. <i>Sustainable Energy and Fuels</i> , 2022, 6, 3756-3767.	2.5	2
12844	Efficient solventless dehydrogenation of formic acid by a CNC-based rhodium catalyst. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 4538-4547.	3.0	8
12845	DFT modelling studies of spectroscopic properties and Medium Effects on Molecular Reactivity of Secnidazole in different solvents. <i>Journal of Physical Chemistry and Functional Materials</i> ; 0, , .	0.0	0
12846	Linear Free Energy Relationships in Electrostatic Catalysis. <i>ACS Catalysis</i> , 2022, 12, 8237-8241.	5.5	5
12847	A local hybrid exchange functional approximation from first principles. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	18
12848	Wide Nematogenic Azomethine/Ester Liquid Crystals Based on New Biphenyl Derivatives: Mesomorphic and Computational Studies. <i>Molecules</i> , 2022, 27, 4150.	1.7	18
12849	Biomolecule-Compatible Dehydrogenative Chan-Lam Coupling of Free Sulfilimines. <i>Journal of the American Chemical Society</i> , 2022, 144, 12476-12487.	6.6	18
12850	Identifying Vibrations that Control Non-adiabatic Relaxation of Polaritons in Strongly Coupled Molecule-Cavity Systems. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6259-6267.	2.1	10
12851	Origin of the Unusual Ground-State Spin $S = 9$ in a Cr ₁₀ Single-Molecule Magnet. <i>Journal of the American Chemical Society</i> , 2022, 144, 12520-12535.	6.6	3
12852	ChASE. , 2022, , .		0
12853	Kinetics study of the OH+SiH ₄ hydrogen abstraction reaction: A theoretical analysis. <i>International Journal of Chemical Kinetics</i> , 0, , .	1.0	0

#	ARTICLE	IF	CITATIONS
12854	Benchmarking time-dependent density functional theory predictions of emission spectra and color: A rainbow of error. <i>International Journal of Quantum Chemistry</i> , 0, .	1.0	1
12855	Bir Florlu Aminoimidazolin Olan Midaflur'un Karbon İyot Kuantum Kimyasal Analizi. <i>Bilecik Şeyh Edebali Üniversitesi Fen Bilimleri Dergisi</i> , 0, .	0.1	0
12856	Not That DDT: A Databank of Dynamics Trajectories for Organic Reactions. <i>Journal of Chemical Education</i> , 2022, 99, 2721-2725.	1.1	4
12857	Construction of a Few-Layered COF@CNT Composite as an Ultrahigh Rate Cathode for Low-Cost K-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 31234-31244.	4.0	22
12858	Theoretical study of the stereoselectivity in the reaction of 4-haloglutamic acid derivatives with arylamines. <i>Russian Chemical Bulletin</i> , 2022, 71, 1135-1142.	0.4	2
12859	Exploring the Protein Tyrosine Phosphatase 1B Inhibitory Potentials of Naturally Occurring Brazilin-Type Isoflavonoids: A Computational Approach. <i>Chemistry Africa</i> , 2022, 5, 1493-1502.	1.2	5
12860	Exploring the Electrochemistry of Iron Dithiolene and Its Potential for Electrochemical Homogeneous Carbon Dioxide Reduction. <i>ChemElectroChem</i> , 2022, 9, .	1.7	1
12861	Correspondence on "How Aromatic Are Molecular Nanorings? The Case of a Six-Porphyrin Nanoring". <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	11
12862	Correspondence on "How Aromatic Are Molecular Nanorings? The Case of a Six-Porphyrin Nanoring". <i>Angewandte Chemie</i> , 0, .	1.6	3
12863	Cyclometalated Platinum(II) Metallomesogens Based on Half-Disc-Shaped β^2 -Diketonate Ligands with Hexacatenar: Crystal Structures, Mesophase Properties, and Semiconductor Devices. <i>Inorganic Chemistry</i> , 2022, 61, 11702-11714.	1.9	4
12864	Benzophenanthrothiophene based donor-acceptor organic dyes for efficient solar cells with long-term stability. <i>Dyes and Pigments</i> , 2022, 205, 110575.	2.0	0
12865	Improving the Accuracy of Composite Methods: A G4MP2 Method with G4-like Accuracy and Implications for Machine Learning. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4528-4536.	1.1	3
12866	Penetration of Nonenergetic Hydrogen Atoms into Amorphous Solid Water and their Reaction with Embedded Benzene and Naphthalene. <i>Astrophysical Journal</i> , 2022, 933, 138.	1.6	2
12867	Synthesis, Crystal Structures, and Density Functional Theory Studies of Two Salt Cocrystals Containing Meldrum's Acid Group. <i>ACS Omega</i> , 2022, 7, 25132-25139.	1.6	3
12868	Ab initio composite strategies and multireference approaches for lanthanide sulfides and selenides. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	6
12869	On the Origin of Photoluminescence Enhancement in Bicosahedral Ag _x Au ₂₅ Nanoclusters (x=13) and Their Application to Triplet-Triplet Annihilation Photon Upconversion. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	13
12870	Nonconventional NMR Spin-Coupling Constants in Oligosaccharide Conformational Modeling: Structural Dependencies Determined from Density Functional Theory Calculations. <i>ACS Omega</i> , 2022, 7, 23950-23966.	1.6	4
12871	Single Ti ³⁺ Ion Catalyzes NO Reduction on Stoichiometric Titanium Oxide Cluster Anions (Ti ₂) _n (n = 1-11). <i>ACS Catalysis</i> , 2022, 12, 8768-8775.	5.5	6

#	ARTICLE	IF	CITATIONS
12891	Experimental, DFT and Theoretical Corrosion Study for 4-(((4-ethyl-5-(thiophen-2-yl)-4H-1,2,4-triazole-3-yl)thio)methyl)-7,8-dimethyl-2H-chromen-2-one. <i>Arabian Journal of Chemistry</i> , 2022, 15, 104088.	2.3	16
12892	Two-dimensional ZnO/MoSe ₂ van der Waals heterostructure used as promising photocatalyst for water splitting: A DFT study. <i>Chemical Physics Letters</i> , 2022, 803, 139828.	1.2	5
12893	Structural and elastic behaviour of aragonite at high-pressure: A contribution from first-principle simulations. <i>Computational Materials Science</i> , 2022, 212, 111600.	1.4	3
12894	A water-soluble manganese(II) octanedioate/phenanthroline complex acts as an antioxidant and attenuates alpha-synuclein toxicity. <i>Biochimica Et Biophysica Acta - Molecular Basis of Disease</i> , 2022, 1868, 166475.	1.8	1
12895	Quantifying the anion effect of gas solubility within ionic liquids using the solvation affinity index. <i>Chemical Engineering Science</i> , 2022, 260, 117851.	1.9	2
12896	Ab initio modeling of helical polyacetylenes: Peierls and Mott-Hubbard metal-insulator transitions. <i>Computational Materials Science</i> , 2022, 213, 111642.	1.4	5
12897	Iron-containing metal-organic framework thin film as a drug delivery system. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 650, 129611.	2.3	9
12898	π-Stacked (C _n -C ₆ H ₆ -Fe-C ₆ H ₆ -C _{13-n}) _{n=2} : A spin operated thermoelectric nanodevice. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 170, 110900.	1.9	0
12899	Quantum chemistry study of the multiphoton absorption in enhanced green fluorescent protein at the single amino acid residue level. <i>ChemPhysChem</i> , 0, , .	1.0	1
12900	Role of dopants in tuning spintronic features of lithium doped g-C ₄ N ₃ @Li _{n=1 to 4} . <i>Journal of Physics: Conference Series</i> , 2022, 2286, 012008.	0.3	0
12901	A unique colorimetric and ratiometric reversible fluorescent probe for HSO ₃ ⁻ /H ₂ O ₂ detection and imaging in real water samples, rice leaves and roots. <i>Dyes and Pigments</i> , 2022, 205, 110591.	2.0	7
12902	Photochemical and Molecular Dynamics Studies of Halide Binding in Flavoenzyme Glucose Oxidase. <i>ChemBioChem</i> , 2022, 23, .	1.3	1
12903	Fullerenes Pose a Strain on Hybrid Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4709-4720.	1.1	5
12904	Bucket Effect to Improve Third-Order Nonlinear Optical Response on Metal-Heteroaromatic Compounds. <i>Chinese Journal of Chemistry</i> , 2022, 40, 2611-2617.	2.6	6
12905	Synthesis, characterization, molecular docking and molecular dynamics simulations of benzamide derivatives as potential anti-ovarian cancer agents. <i>Journal of Molecular Structure</i> , 2022, 1269, 133785.	1.8	32
12906	Unveiling the sensing mechanism and luminescence property of a new ESIPT-based fluorescent sensor for detecting Zn ²⁺ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 282, 121650.	2.0	16
12907	A Theoretical Study of Infrared Spectra of Highly Positively Charged C ₆₀ Fullerenes and Their Relevance to Observed UIE Features. <i>Astrophysical Journal</i> , 2022, 934, 75.	1.6	3
12908	Proton-transfer reactions of Re(II)-nitrosyl complexes: Potentiometric studies, DFT and TD-DFT calculations. <i>Results in Chemistry</i> , 2022, 4, 100455.	0.9	1

#	ARTICLE	IF	CITATIONS
12909	Study by DFT of the functionalization of amylose/amylopectin with glycerin monoacetate: Characterization by FTIR, electronic and adsorption properties. <i>Journal of Molecular Structure</i> , 2022, 1269, 133761.	1.8	5
12910	Theoretical studies on boron dimethyl-based thermally activated delayed fluorescence organic emitters: excited-state properties and mechanisms. <i>New Journal of Chemistry</i> , 2022, 46, 15678-15685.	1.4	1
12911	Fluoride ion coordination-induced turn-on fluorescence of tailored <i>N</i> -methyl <i>N</i> -confused tripyrromethene analogues. <i>Organic and Biomolecular Chemistry</i> , 0, , .	1.5	0
12912	A litmus test for the balanced description of dispersion interactions and coordination chemistry of lanthanoids. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1
12913	Decisive role of heavy-atom orientation for efficient enhancement of spin-orbit coupling in organic thermally activated delayed fluorescence emitters. <i>Journal of Materials Chemistry C</i> , 2022, 10, 11719-11729.	2.7	5
12914	Stable, Bright, and Long-Fluorescence-Lifetime Dyes for Deep-Near-Infrared Bioimaging. <i>Journal of the American Chemical Society</i> , 2022, 144, 14351-14362.	6.6	65
12915	The Distance between Minima of Electron Density and Electrostatic Potential as a Measure of Halogen Bond Strength. <i>Molecules</i> , 2022, 27, 4848.	1.7	7
12916	Synthesis of Two Novel Copper (II) Complexes as Potential Inhibitors of HIV-1 Protease Enzyme: Experimental and Theoretical Investigations. <i>Crystals</i> , 2022, 12, 1066.	1.0	3
12917	Targeting the Major Groove of the Palindromic d(GCGCC) ₂ Sequence by Oligopeptide Derivatives of Anthraquinone Intercalators. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 6649-6666.	2.5	3
12918	Recent Advances in Cartesian-Grid DFT in Atoms and Molecules. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	0
12919	Insights into the Design of An Enzyme Free Sustainable Sensing Platform for Efavirenz. <i>Catalysts</i> , 2022, 12, 830.	1.6	2
12920	Theoretical estimates of sulfoxanion triple-oxygen equilibrium isotope effects and their implications. <i>Geochimica Et Cosmochimica Acta</i> , 2022, 336, 353-371.	1.6	2
12921	Computation of NMR shieldings at the CASSCF level using gauge-including atomic orbitals and Cholesky decomposition. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	4
12922	Theoretical study of keto-enol tautomerism in 7-epi-clusianone by quantum chemical calculations of NMR chemical shifts. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	1
12923	Theoretical Investigations of the OH-Initiated Oxidation of 4-Methyl-3-Penten-2-One in the Atmosphere. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 2261-2273.	1.2	1
12924	Substituent Control of Near-Infrared Absorption of Triphenylamine Radical Cation. <i>Colorants</i> , 2022, 1, 354-362.	0.9	1
12925	Ruthenium (II) Complexes Bearing <i>N</i> -Heterocyclic Carbene Based C ^N Donor Sets in Dye-Sensitized Solar Cells. <i>Applied Organometallic Chemistry</i> , 0, , .	1.7	1
12926	Investigation of the Solution Chemistry of Hybrid Organic-Inorganic Indium Halides for New Material Discovery. <i>Inorganic Chemistry</i> , 2022, 61, 13015-13021.	1.9	3

#	ARTICLE	IF	CITATIONS
12927	Unusually Large Effects of Charge-Assisted C-H...F Hydrogen Bonds to Anionic Fluorine in Organic Solvents: Computational Study of ¹⁹ F NMR Shifts versus Thermochemistry. <i>ChemistryOpen</i> , 2022, 11, .	0.9	4
12928	Intramolecular force field for carboxylate Pt(II)-complexes. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	1
12930	Quenching singlet oxygen via intersystem crossing for a stable Li-O ₂ battery. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	20
12931	Grain-Surface Hydrogen-Addition Reactions as a Chemical Link Between Cold Cores and Hot Corinos: The Case of H ₂ CCS and CH ₃ CH ₂ SH. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5343-5353.	1.1	4
12932	Enabling <i>Ab Initio</i> Material Design of $\ln\text{As}$ Superlattices for Infrared Detection. <i>Physical Review Applied</i> , 2022, 18, .	1.5	1
12933	Vibrational Circular Dichroism Unravels Supramolecular Chirality and Hydration Polymorphism of Nucleoside Crystals. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	9
12934	Balanced Interfacial Ion Concentration and Migration Steric Hindrance Promoting High-Efficiency Deposition/Dissolution Battery Chemistry. <i>Advanced Materials</i> , 2022, 34, .	11.1	48
12935	Water-Facilitated Nitromethane-Mediated Cyclization of 2-(Phenylvinyl)benzhydrols: Access to 1,3-Diphenyl-1H-indenes with Antitumor Activity. <i>Advanced Synthesis and Catalysis</i> , 2022, 364, 3004-3015.	2.1	0
12937	Analysis of protein structures containing <i>HEPES</i> and <i>MES</i> molecules. <i>Protein Science</i> , 2022, 31, .	3.1	0
12938	Computational investigation of isoeugenol transformations on a platinum cluster μ_4 : Direct deoxygenation to propylcyclohexane. <i>Molecular Catalysis</i> , 2022, 529, 112541.	1.0	1
12939	The chemistry of AlF and CaF production in buffer gas sources. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	3
12940	Benefits of Range-Separated Hybrid and Double-Hybrid Functionals for a Large and Diverse Data Set of Reaction Energies and Barrier Heights. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5492-5505.	1.1	11
12941	London Disperse Interactions Assist Chiral Induction in the Soai Autoamplifying Reaction Provoked by 1- and 2-Aza[6]helicenes. <i>Catalysts</i> , 2022, 12, 859.	1.6	1
12942	Koopmans Spectral Functionals in Periodic Boundary Conditions. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 5435-5448.	2.3	6
12943	Theoretical Investigation of the Biogenetic Pathway for Formation of Antibacterial Indole Alkaloids from <i>Voacanga africana</i> . <i>ACS Omega</i> , 2022, 7, 31591-31596.	1.6	3
12944	Theoretical Mechanistic Studies of the Polymerization of Functionalized Styrenes Catalyzed by Rare-Earth-Metal Complexes: Stereoselectivity Regulation. <i>Organometallics</i> , 2022, 41, 2466-2473.	1.1	3
12945	Efficient simulation of resonance Raman spectra with tight-binding approximations to density functional theory. <i>Journal of Chemical Physics</i> , 2022, 157, 084104.	1.2	1
12946	Understanding structure-properties relationships of porphyrin linked to graphene oxide through π - π -stacking or covalent amide bonds. <i>Scientific Reports</i> , 2022, 12, .	1.6	6

#	ARTICLE	IF	CITATIONS
12947	Acid Rain and Flue Gas: Quantum Chemical Hydrolysis of NO ₂ . ChemPhysChem, 0, , .	1.0	6
12948	Stereoconvergent Synthesis of Cyclopentenyl Nucleosides by Palladium-Assisted Allylic Reaction. European Journal of Organic Chemistry, 0, , .	1.2	1
12949	Binding energy analysis and molecular dynamic simulation studies of the designed orally active, non-toxic GABARAP modulators. Journal of Biomolecular Structure and Dynamics, 2023, 41, 6394-6412.	2.0	1
12950	Why Ortho- and Para-Hydroxy Metabolites Can Scavenge Free Radicals That the Parent Atorvastatin Cannot? Important Pharmacologic Insight from Quantum Chemistry. Molecules, 2022, 27, 5036.	1.7	4
12951	DFT rationalization of metal-catalyst-controlled coupling of carbazole with diazo-naphthalen-2(1H)-one. Molecular Catalysis, 2022, 529, 112574.	1.0	1
12952	A Computational Protocol for Vibrational Circular Dichroism Spectra of Cyclic Oligopeptides. Journal of Physical Chemistry A, 2022, 126, 5458-5471.	1.1	11
12953	Band-gap engineering of rutile-structured SnO_2 alloy system. Physical Review Materials, 2022, 6, .	1.0	1
12954	Nonlinear optical properties DFT calculations of polyacetylene and copolymers models substituted with aldimines chromophores as side chains. Journal of Computational Chemistry, 2022, 43, 1701-1718.	1.5	2
12956	Carbene-Like Reactivity in an Iron Azametallacyclobutene Complex: Insights from Electronic Structure. Inorganic Chemistry, 2022, 61, 13266-13270.	1.9	3
12957	Vibronic fine structure in the nitrogen photoelectron spectra of molecules from Franck-Condon simulations: Azines. Physical Review A, 2022, 106, .	1.0	4
12958	Caught while Dissolving: Revealing the Interfacial Solvation of the Mg ²⁺ Ions on the MgO Surface. ACS Applied Materials & Interfaces, 2022, 14, 38370-38378.	4.0	7
12959	Quantum chemical design of near-infrared retinal-based pigments and evaluating their vibronic/electronic properties. Computational and Theoretical Chemistry, 2022, 1215, 113835.	1.1	0
12960	TMP/Pd complex immobilized on graphene oxide for efficient pseudocapacitive energy storage with combined experimental and DFT study. Journal of Molecular Liquids, 2022, 364, 120008.	2.3	0
12961	Crystallographic studies of fac- and mer-isomers of Cu[1,4,7,10,13,16-hexaazacyclooctadecane] ²⁺ . Influence of counterion and crystallization solvent on crystal structure and dynamic Jahn-Teller effects. Computational studies of structures, energetics, and mechanism of mer-fac isomerization. Polyhedron, 2022, 225, 116072.	1.0	0
12962	Electronic structure calculations of the fundamental interactions in solvent extraction desalination. Journal of Molecular Liquids, 2022, 364, 119986.	2.3	6
12963	A DFT+U approach to doped SrTiO ₃ for solar harvesting applications. Computational Materials Science, 2022, 214, 111743.	1.4	6
12964	Spectro-electrochemical, fluorometric and biothermodynamic evaluation of pharmacologically active morpholine scaffold single crystal ligand and its metal(II) complexes: A comparative study on in-vitro and in-silico screening towards DNA/BSA/SARS-CoV-19. Journal of Inorganic Biochemistry, 2022, 236, 111953.	1.5	8
12965	Electronic interaction between two fluorenyl-bridged molybdenocene dithiolene electroactive centers. Polyhedron, 2022, 226, 116086.	1.0	1

#	ARTICLE	IF	CITATIONS
12966	Synthesis, photophysical, electrochemical and computational investigation of dimethine and trimethine cyanine-based dyes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 433, 114189.	2.0	6
12967	Molecular dynamics simulation on water/oil interface with model asphaltene subjected to electric field. <i>Journal of Colloid and Interface Science</i> , 2022, 628, 924-934.	5.0	9
12968	Synthesis, characterization, DFT, QSAR, antimicrobial, and antitumor studies of some novel pyridopyrimidines. <i>Journal of Molecular Structure</i> , 2022, 1269, 133870.	1.8	11
12969	Structural, spectroscopic and computational studies of two new spirocompounds containing 2,3,4-trimethoxybenzyl group. <i>Journal of Molecular Structure</i> , 2022, 1269, 133806.	1.8	3
12970	Design, synthesis, bioevaluation, DFT, docking, and molecular dynamic simulation for selected novel 1,3,4-Oxadiazole - indole derivatives hybrid against estrogen receptor alpha. <i>Journal of Molecular Structure</i> , 2022, 1269, 133789.	1.8	4
12971	Modeling Hydrogen and Oxygen Evolution Reactions on Single Atom Catalysts with Density Functional Theory: Role of the Functional. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	20
12972	Quantum chemical studies on the binding domain of SARS-CoV-2 S-protein: human ACE2 interface complex. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 7354-7364.	2.0	1
12973	Ultrafast charge-transfer dynamics in a visible-light-excited iridium(III) terpyridine 2-phenylpyridine complex studied by femtosecond X-ray absorption spectroscopy. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 435, 114267.	2.0	0
12974	Bipolar tetraphenylsilane-based host molecules for blue phosphorescence. <i>Dyes and Pigments</i> , 2022, 206, 110684.	2.0	0
12975	Insights into solvent effects on molecular properties, physicochemical parameters, and NLO behavior of brinzolamide, a bioactive sulfonamide: A computational study. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100738.	1.3	5
12976	First-principles investigation of Hydroxycarbamide anticancer drug delivery by X12N12 (X=Al, Ga) fullerene nanostructures: A DFT, NBO and QTAIM analysis. <i>Computational and Theoretical Chemistry</i> , 2022, 1216, 113869.	1.1	4
12977	Synthesis and application of chloroacetamides in pyridinium based ionic liquid for high temperature extraction of uranyl ion: A novel and 'green' approach for extractive mass transfer at elevated temperature. <i>Journal of Molecular Liquids</i> , 2022, 365, 120222.	2.3	1
12978	Assessment of seventeen density functionals to estimate the global reactivity of C20 in the framework of the conceptual density functional theory. <i>Chemical Physics Letters</i> , 2022, 806, 140005.	1.2	1
12979	Reactivity of oxo- and thiophosphonium Lewis acids towards acetonitrile and pyridine. <i>Polyhedron</i> , 2022, 227, 116138.	1.0	1
12980	Synthesis and performance of two ecofriendly epoxy resins as a highly efficient corrosion inhibition for carbon steel in 1M HCl solution: DFT, RDF, FFV and MD approaches. <i>Chemical Physics Letters</i> , 2022, 806, 139995.	1.2	29
12981	Nitrobenzamido substitution on thiophene-3-carboxylate: Electrochemical investigation, antioxidant activity, molecular docking, DFT calculations. <i>Journal of Molecular Structure</i> , 2023, 1271, 134030.	1.8	13
12982	Structural and photoelectrochemical dynamics of in-situ hydrogenated anatase TiO2 thin films grown by DC reactive magnetron sputtering. <i>Applied Surface Science</i> , 2023, 607, 155023.	3.1	3
12983	Chemical warfare agents: an outlook on past and present technologies. , 2023, , 3-31.		1

#	ARTICLE	IF	CITATIONS
12984	Dynamics of electron collision with potential biofuel: N-butanol. Radiation Physics and Chemistry, 2023, 202, 110504.	1.4	4
12985	Density-functional theory. , 2023, , 27-65.		0
12986	Study on the mechanism of free radical scavenger TEMPO blocking in coal oxidation chain reaction. Fuel, 2023, 331, 125853.	3.4	12
12987	Experimental and theoretical studies on naphthalene based fluorophores: Applications in detection of Al ³⁺ ions in water, soil, food and live cells. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 435, 114268.	2.0	6
12988	The resolution- <i>vs.</i> -accuracy dilemma in machine learning modeling of electronic excitation spectra. , 2022, 1, 689-702.		4
12989	Study on the Mechanism of Free Radical Trapping Agent Tempo Blocking in Coal Oxidation Chain Reaction. SSRN Electronic Journal, 0, , .	0.4	0
12990	DFT studies on rhodium(ⁱⁱⁱ)-catalyzed synthesis of indanones from <i>N</i> -methoxybenzamides <i>via</i> C-H activation reaction. New Journal of Chemistry, 2022, 46, 16576-16583.	1.4	0
12991	A solvent-mediated conformational switch in sulfanilamide. Physical Chemistry Chemical Physics, 2022, 24, 24032-24038.	1.3	2
12992	Realization of switching between TADF and HLCT emissions through modulation of the intramolecular charge transfer character. Journal of Materials Chemistry C, 2022, 10, 13124-13136.	2.7	8
12993	Pericyclic reaction benchmarks: hierarchical computations targeting CCSDT(Q)/CBS and analysis of DFT performance. Physical Chemistry Chemical Physics, 2022, 24, 18028-18042.	1.3	14
12994	Revealing the Acetylcholinesterase Inhibitory Potential of <i>Phyllanthus amarus</i> and Its Phytoconstituents: In Vitro and in Silico Approach. Bioinformatics and Biology Insights, 2022, 16, 117793222211183.	1.0	3
12995	Density Functional Theory on the CO ₂ Absorption Process with Ionic Liquids. Computer Aided Chemical Engineering, 2022, , 967-972.	0.3	0
12996	Synthesis and characterisation of group 8 tris(1-benzyl-1,2,3-triazol-4-yl)- <i>p</i> -anisolylmethane complexes. Dalton Transactions, 2022, 51, 13692-13702.	1.6	0
12997	The role of the intermediate triplet state in iron-catalyzed multi-state C-H activation. Physical Chemistry Chemical Physics, 2022, 24, 20721-20727.	1.3	1
12998	Evaluating the impact of Hartree-Fock exact exchange on the performance of global hybrid functionals for the vertical excited-state energies of fused-ring electron acceptors using TD-DFT. Physical Chemistry Chemical Physics, 2022, 24, 21270-21282.	1.3	1
12999	Geometric requirements for living anionic polymerization: polymerization of rotationally constrained 1,3-dienes. Polymer Chemistry, 2022, 13, 5478-5485.	1.9	3
13000	Experimental and theoretical investigations on three Dy ^{III} ₄ single molecule magnets: structural and magneto-structural correlations. Dalton Transactions, 2022, 51, 14753-14766.	1.6	1
13001	From vibrational spectroscopy and quantum tunnelling to periodic band structures – a self-supervised, all-purpose neural network approach to general quantum problems. Physical Chemistry Chemical Physics, 2022, 24, 25191-25202.	1.3	3

#	ARTICLE	IF	CITATIONS
13002	The smallest 4f-metalla-aromatic molecule of cyclo-PrB ₂ ⁺ with Pr ⁺ B multiple bonds. <i>Chemical Science</i> , 2022, 13, 10082-10094.	3.7	4
13003	Energy Decomposition Analysis of the Chemical Bond: Scope and Limitation. , 2024, , 322-361.		6
13004	A Theoretical Investigation of the Possible Mechanisms for Detection the Copper Ions by a Retinal-Base Sensor. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
13005	The S ⁺ +SiH ₂ Reaction: Toward the Synthesis of Interstellar SiS. <i>Lecture Notes in Computer Science</i> , 2022, , 233-245.	1.0	1
13006	Low-frequency Raman optical activity provides insight into the structure of chiral liquids. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 19722-19733.	1.3	6
13007	A metal complex based fluorescent chemodosimeter for selective detection of 2,4-dinitrophenol and picric acid in aqueous media. <i>Dalton Transactions</i> , 2022, 51, 14700-14711.	1.6	2
13008	<i>In silico</i> activation of dinitrogen with a light atom molecule. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20953-20967.	1.3	3
13009	Synthesis, crystal structure, EPR, and DFT studies of an unusually distorted vanadium(<i>ii</i>) complex. <i>Dalton Transactions</i> , 2022, 51, 12031-12036.	1.6	0
13010	Reactivity of Oxo- and Thiophosphonium Lewis Acids Towards Acetonitrile and Pyridine. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
13011	A multi-technique approach to unveil the redox behaviour and potentiality of homoleptic Cu ^I complexes based on substituted bipyridine ligands in oxygenation reactions. <i>Dalton Transactions</i> , 2022, 51, 14439-14451.	1.6	1
13012	Reaction mechanism of the <i>Pu</i> dimethylsulfoniopropionate lyase and cofactor effects of various transition metal ions. <i>Dalton Transactions</i> , 2022, 51, 14664-14672.	1.6	0
13013	Fragmentation of interstellar methanol by collisions with He ⁺ : an experimental and computational study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 22437-22452.	1.3	5
13014	Existence of noble gas-inserted phosphorus fluorides: FN ₂ PF ₄ and FNPF ₄ with Ng ⁺ P covalent bond (Ng = Ar, Kr, Xe and Rn). <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20466-20479.	1.3	2
13015	Non-Aufbau orbital ordering and spin density modulation in high-spin donor-acceptor conjugated polymers. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 23699-23711.	1.3	4
13016	Gas-phase spectroscopic identification of the chlorovinyl radical. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 25099-25105.	1.3	1
13017	Carboxylate binding prefers two cations to one. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 22198-22205.	1.3	4
13018	Computational exploration for possible reaction pathways, regioselectivity, and influence of substrate in gold-catalyzed cycloaddition of cyanamides with enynamides. <i>RSC Advances</i> , 2022, 12, 22939-22945.	1.7	0
13019	On the origin of the inverted singlet-triplet gap of the 5th generation light-emitting molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18713-18721.	1.3	23

#	ARTICLE	IF	CITATIONS
13020	Intramolecular Hydrogen Bonding Patterns and Conformational Preferences of Ouabain—A Molecule with Cardiotoxic and Antiviral Activities. <i>Engineering Materials</i> , 2022, , 671-696.	0.3	0
13021	DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 28700-28781.	1.3	91
13022	Silica dimerization in the presence of divalent cations. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 21308-21320.	1.3	5
13023	Newly identified C—H...O hydrogen bond in histidine. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 19233-19251.	1.3	2
13024	<i>In silico</i> capture of noble gas atoms with a light atom molecule. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20968-20979.	1.3	2
13025	Theory and Computation in Photo-Electro-Chemical Catalysis: Highlights, Challenges, and Prospects. <i>Engineering Materials</i> , 2022, , 3-43.	0.3	0
13026	Using diketopyrrolopyrroles to stabilize double excitation and control internal conversion. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 23279-23288.	1.3	2
13027	Density Functional Theory. , 2022, , 1-16.		0
13028	A Theoretical Investigation of the Reactions of N_2 and CN with Acrylonitrile and Implications for the Prebiotic Chemistry of Titan. <i>Lecture Notes in Computer Science</i> , 2022, , 246-259.	1.0	0
13029	Green synthesis of gold nanoparticles using quercetin biomolecule from mangrove plant, <i>Cerriops tagal</i> : Assessment of antiproliferative properties, cellular uptake and DFT studies. <i>Journal of Molecular Structure</i> , 2023, 1272, 134167.	1.8	6
13031	Computational Assessment of Xanthenes from African Medicinal Plants as Aldose Reductase Inhibitors. <i>Computation</i> , 2022, 10, 146.	1.0	5
13032	Identification of the Catalytically Dominant Iron Environment in Iron- and Nitrogen-Doped Carbon Catalysts for the Oxygen Reduction Reaction. <i>Journal of the American Chemical Society</i> , 2022, 144, 16827-16840.	6.6	35
13033	Acetaldehyde binding energies: a coupled experimental and theoretical study. <i>Monthly Notices of the Royal Astronomical Society</i> , 2022, 516, 2586-2596.	1.6	8
13034	New Deferric Amine Compounds Efficiently Chelate Excess Iron to Treat Iron Overload Disorders and to Prevent Ferroptosis. <i>Advanced Science</i> , 2022, 9, .	5.6	15
13035	First-Principles Study of Cu-Based Inorganic Hole Transport Materials for Solar Cell Applications. <i>Materials</i> , 2022, 15, 5703.	1.3	1
13037	Comparative Interaction Studies of Quercetin with 2-Hydroxyl-propyl- β -cyclodextrin and 2,6-Methylated- β -cyclodextrin. <i>Molecules</i> , 2022, 27, 5490.	1.7	7
13038	Zinc oxide nanoclusters and their potential application as CH_4 and CO_2 gas sensors: Insight from DFT and TD-DFT. <i>Journal of Computational Chemistry</i> , 2022, 43, 1839-1847.	1.5	11
13039	A QM/MM Study on the X-ray Spectra of Organic Proton Transfer Crystals of Isonicotinamides. <i>Journal of Physical Chemistry C</i> , 2022, 126, 15849-15863.	1.5	9

#	ARTICLE	IF	CITATIONS
13040	Gallium(III)-pyridoxal thiosemicarbazone derivatives as nontoxic agents against Gram-negative bacteria. <i>Metallomics</i> , 2022, 14, .	1.0	4
13041	Modeling X-ray Photoelectron Spectroscopy of Macromolecules Using <i>GW</i> . <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 8666-8672.	2.1	7
13042	Accurate Vertical Excitation Energies of BODIPY/Aza-BODIPY Derivatives from Excited-State Mean-Field Calculations. <i>Journal of Physical Chemistry A</i> , 0, , .	1.1	5
13043	Ligand Rotation Induced Oxidation State Change and Spin Appearance of the Bis(phthalocyaninato)cerium (CePc ₂) Molecule on the Au(111) Surface. <i>Journal of Physical Chemistry C</i> , 2022, 126, 17152-17163.	1.5	0
13044	Thermodynamics and dielectric response of BaTiO ₃ by data-driven modeling. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	15
13045	Homoatomic cations: From [P ₅] ⁺ to [P ₉] ⁺ . <i>Science Advances</i> , 2022, 8, .	4.7	4
13046	Antioxidant and anticancer properties of plant-based bioactive flavonoids cardamomin and alpinetin: A theoretical insight from H^{\bullet} OOH antiradical and Cu (II) chelation mechanisms. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	2
13047	Prophylactic and Therapeutic Potential Zinc Metallodrugs Drug Discovery: Identification of SARS-CoV-2 Replication and Spike/ACE2 Inhibitors. <i>Current Computer-Aided Drug Design</i> , 2022, 18, 519-534.	0.8	1
13048	Chemical and Redox Speciation of Uranyl with Three Environmentally Relevant Bifunctional Chelates: Multi-Technique Approach Combined with Theoretical Estimations. <i>Inorganic Chemistry</i> , 2022, 61, 15452-15462.	1.9	2
13049	An initial investigation of accuracy required for the identification of small molecules in complex samples using quantum chemical calculated NMR chemical shifts. <i>Journal of Cheminformatics</i> , 2022, 14, .	2.8	0
13050	The performance of exchange correlation functionals in describing electron density parameters of saddle point structures along chemical reactions. <i>Journal of Computational Chemistry</i> , 2022, 43, 1830-1838.	1.5	1
13051	Computational Evaluation of Potential Molecular Catalysts for Nitrous Oxide Decomposition. <i>Inorganic Chemistry</i> , 2022, 61, 14591-14605.	1.9	2
13052	Reaction N ₂ D + CH ₂ CCH ₂ (Allene): An Experimental and Theoretical Investigation and Implications for the Photochemical Models of Titan. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 2305-2321.	1.2	6
13053	Conformational Heterogeneity and Interchain Percolation Revealed in an Amorphous Conjugated Polymer. <i>ACS Nano</i> , 2022, 16, 14432-14442.	7.3	4
13055	Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory for Accurate X-ray Absorption Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 6240-6250.	2.3	5
13056	Designing a 0D/1D S-Scheme Heterojunction of Cadmium Selenide and Polymeric Carbon Nitride for Photocatalytic Water Splitting and Carbon Dioxide Reduction. <i>Molecules</i> , 2022, 27, 6286.	1.7	4
13057	The N ₂ D + CH ₂ CHCN (Vinyl Cyanide) Reaction: A Combined Crossed Molecular Beam and Theoretical Study and Implications for the Atmosphere of Titan. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6110-6123.	1.1	10
13058	Pyramid-Like Au ₂ -CNC under an External Electric Field: Charge Transfer, UV-Vis Absorption Spectra, and Nonlinear Optical Property. <i>Journal of Physical Chemistry C</i> , 2022, 126, 16236-16242.	1.5	4

#	ARTICLE	IF	CITATIONS
13059	Atmospheric Oxidation of Imine Derivative of Piperazine Initiated by OH Radical. ACS Earth and Space Chemistry, 2022, 6, 2453-2464.	1.2	6
13060	Local Hybrid Functional Applicable to Weakly and Strongly Correlated Systems. Journal of Chemical Theory and Computation, 2022, 18, 6111-6123.	2.3	11
13061	Thorough Understanding of Bioluminophore Production in Bacterial Bioluminescence. Journal of Physical Chemistry A, 2022, 126, 6604-6616.	1.1	3
13062	Adsorption of Selected Molecules on (TiO ₂) ₂₀ Nano-Clusters: A Density-Functional-Theory Study. Nanomanufacturing, 2022, 2, 124-145.	1.8	5
13063	C-H Insertion in Dirhodium Tetracarboxylate-Catalyzed Reactions despite Dynamical Tendencies toward Fragmentation: Implications for Reaction Efficiency and Catalyst Design. Journal of the American Chemical Society, 2022, 144, 17219-17231.	6.6	10
13064	An Experimental and Theoretical Investigation of HCN Production in the Hadean Earth Atmosphere. ACS Earth and Space Chemistry, 2022, 6, 2385-2399.	1.2	2
13065	Size-dependent adsorption performance of ZnO nanoclusters for drug delivery applications. Structural Chemistry, 2023, 34, 1061-1071.	1.0	9
13066	Spectroscopy of Retinoic Acid at the Air-Water Interface. Journal of Physical Chemistry A, 2022, 126, 6908-6919.	1.1	4
13067	Enhancing Horizontal Ratio of Transition Dipole Moment in Homoleptic Ir Complexes for High Outcoupling Efficiency of Organic Light-Emitting Diodes. Advanced Science, 2022, 9, .	5.6	8
13068	Probing Optoelectronic and Thermoelectric Properties of Lead-Free Perovskite SnTiO ₃ : HSE06 and Boltzmann Transport Calculations. Crystals, 2022, 12, 1317.	1.0	9
13069	Characterization of Aggregating Agents towards Sensitive Optical Detection of Tryptophan Using Lab-on-a-Chip. Photonics, 2022, 9, 648.	0.9	1
13070	Role of -Substitution on C-H Activation Reactivity of Iron(IV)-Oxo Cyclam Complexes: a Computational Investigation. Inorganic Chemistry, 2022, 61, 14582-14590.	1.9	0
13071	Unraveling the Role of the Tyrosine Tetrad from the Binding Site of the Epigenetic Writer MLL3 in the Catalytic Mechanism and Methylation Multiplicity. International Journal of Molecular Sciences, 2022, 23, 10339.	1.8	2
13072	Revisiting fundamental properties of TiO ₂ nanoclusters as condensation seeds in astrophysical environments. Astronomy and Astrophysics, 2022, 668, A35.	2.1	5
13073	Investigation of the CO releasing ability of azachalcone bound Mn(I) tricarbonyl complexes and their antiproliferative properties. Applied Organometallic Chemistry, 0, , .	1.7	1
13075	Quantum Chemical Investigation, Electronic Properties, Docking, and ADMET Studies on p-(2-Bromoethoxy) Anisole as Breast Cancer Agent. Polycyclic Aromatic Compounds, 2023, 43, 6766-6784.	1.4	1
13076	4-component relativistic Hamiltonian with effective QED potentials for molecular calculations. Journal of Chemical Physics, 2022, 157, .	1.2	17
13077	Computational Protocol to Evaluate Electron-Phonon Interactions Within Density Matrix Perturbation Theory. Journal of Chemical Theory and Computation, 2022, 18, 6031-6042.	2.3	6

#	ARTICLE	IF	CITATIONS
13078	Critical analysis of radical scavenging properties of atorvastatin in methanol recently estimated via density functional theory. Computational and Theoretical Chemistry, 2022, 1217, 113898.	1.1	3
13079	Adsorption of imidazolium-based ionic liquids on the Fe(1 0 0) surface for corrosion inhibition: Physisorption or chemisorption?. Journal of Molecular Liquids, 2022, 367, 120489.	2.3	12
13080	Sequential Bond Dissociation Energies of Th ⁺ (CO) _x , $x = 3-6$: Guided Ion Beam Collision-Induced Dissociation and Quantum Computational Studies. Inorganic Chemistry, 2022, 61, 15936-15952.	1.9	1
13081	Rational Design of a Fluorescent Chromophore as a Calcium Receptor via DFT and Multivariate Approaches. Molecules, 2022, 27, 6248.	1.7	1
13082	Molecular Motion in the Interconverting f-H ₂ , Di-, and Tri-hydride Regimes: Mo(PH ₃) ₅ H ₂ . Journal of Physical Chemistry A, 2022, 126, 6834-6848.	1.1	0
13083	Sulfite-Catalyzed Nucleophilic Substitution Reactions with Thiamin and Analogous Pyrimidine Donors Proceed via an S _N AE Mechanism. Journal of Organic Chemistry, 2022, 87, 13224-13235.	1.7	0
13084	Fast Screening of Minimum Energy Crossing Points with Semiempirical Tight-Binding Methods. Journal of Chemical Theory and Computation, 2022, 18, 6370-6385.	2.3	6
13085	Capturing the ground state of uranium dioxide from first principles: Crystal distortion, magnetic structure, and phonons. Physical Review B, 2022, 106, .	1.1	7
13086	Rapid calculation of internal conversion and intersystem crossing rate for organic materials discovery. Journal of Chemical Physics, 2022, 157, .	1.2	5
13087	Iron-Catalyzed Kumada Cross-Coupling Reaction Involving Fe ₈ Me ₁₂ and Related Clusters: A Computational Study. ACS Catalysis, 2022, 12, 12678-12688.	5.5	0
13088	How good are recent density functionals for ground and excited states of one-electron systems?. Journal of Chemical Physics, 2022, 157, .	1.2	6
13089	Extraordinary piezoelectric effect induced in two-dimensional rare earth monochalcogenides via reducing system dimensionality. Journal of Materiomics, 2023, 9, 72-81.	2.8	4
13090	Alternating 1-Phenyl-2,2,2-Trifluoroethanol Conformational Landscape With the Addition of One Water: Conformations and Large Amplitude Motions. Journal of Physical Chemistry A, 2022, 126, 7250-7260.	1.1	10
13091	General Design Strategy to Precisely Control the Emission of Fluorophores via a Twisted Intramolecular Charge Transfer (TICT) Process. Journal of the American Chemical Society, 2022, 144, 19778-19790.	6.6	41
13092	Revisiting Ligand-Ligand Charge Transfer Phosphorescence Emission from Zinc(II) Diimine Bis-Thiolate Complexes: It is Actually Thermally Activated Delayed Fluorescence. ChemPhotoChem, 2023, 7, .	1.5	11
13093	Aza-PNA: Engineering E-Rotamer Selectivity Directed by Intramolecular H-bonding. Organic Letters, 2022, 24, 7421-7427.	2.4	1
13094	DFT-based computations on some structurally related N-substituted piperazines. Journal of the Indian Chemical Society, 2022, 99, 100766.	1.3	7
13095	Exploring the Fe doped borazine system as a promising CFC adsorbent: A DFT study. Computational and Theoretical Chemistry, 2022, 1217, 113903.	1.1	1

#	ARTICLE	IF	CITATIONS
13096	Dithiocarbamate chelated chloro bridged linear trinuclear rhenium complexes: Synthesis, structure, spectroscopic and computational studies. <i>Results in Chemistry</i> , 2022, 4, 100577.	0.9	0
13097	A new double-reference correction scheme for accurate and efficient computation of NMR chemical shieldings. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 27055-27063.	1.3	3
13098	Interactions of limonene with the water dimer. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26529-26538.	1.3	1
13099	Directed gas phase preparation of ethynylallene ($H_2CCCHCCH$; X^{1+}) via the crossed molecular beam reaction of the methylidyne radical (CH ; X^{2+}) with vinylacetylene ($H_2CCHCCH$; X^{1+}). <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26499-26510.	1.3	3
13100	Q-Band relaxation in chlorophyll: new insights from multireference quantum dynamics. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 27212-27223.	1.3	4
13101	Reversibly switchable methanofullerene by photoexcitation and reduction. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26998-27003.	1.3	2
13102	Effects of Environmental and Electric Perturbations on the pKa of Thioredoxin Cysteine 35: A Computational Study. <i>Molecules</i> , 2022, 27, 6454.	1.7	1
13103	Infrared Reflection-Absorption Spectroscopy of $\hat{I}\pm$ -Hydroxyacids at the Water-Air Interface. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8280-8294.	1.1	5
13104	Proton-Coupled, Low-Energy Pathway for Electrocatalytic CO_2 Reduction at Re (Diimine) Complexes with a Conjugated Pyrazinyl Moiety. <i>Inorganic Chemistry</i> , 2022, 61, 17505-17514.	1.9	5
13105	Chemical bonding in representative astrophysically relevant neutral, cation, and anion HC_nH chains. <i>Chinese Physics B</i> , 2022, 31, 123101.	0.7	2
13106	Superstrong Chemical Bonding of Noble Gases with Oxidoboron (BO^{++}) and Sulfidoboron (BS^{++}). <i>Journal of Physical Chemistry A</i> , 2022, 126, 7888-7900.	1.1	3
13108	Theoretical study of infrared and ultraviolet spectra of fourteen isomers of C_{24} and comparison with astronomical observations. <i>Monthly Notices of the Royal Astronomical Society</i> , 0, , .	1.6	0
13109	Influence of the CN Orientation on the Degree of Electron Delocalization of $Ru^{\text{II}}Ru^{\text{III}}$ Mixed-Valent Complexes. <i>Inorganic Chemistry</i> , 0, , .	1.9	3
13110	Rotation-Inversion Isomerization of Tertiary Carbamates: Potential Energy Surface Analysis of Multi-Paths Isomerization Using Boltzmann Statistics. <i>ChemPhysChem</i> , 2023, 24, .	1.0	1
13111	Towards the engineering of a photon-only two-stroke rotary molecular motor. <i>Nature Communications</i> , 2022, 13, .	5.8	13
13112	Unification of Perdew-Zunger self-interaction correction, DFT+U, and Rung 3.5 density functionals. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	3
13113	Modeling of excited state potential energy surfaces with the Bethe-Salpeter equation formalism: The 4-(dimethylamino)benzonitrile twist. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	9
13114	An Integrated Experimental and Theoretical Studies on the Corrosion Inhibition of Carbon Steel by Harmful Extracts. <i>Molecules</i> , 2022, 27, 7250.	1.7	4

#	ARTICLE	IF	CITATIONS
13115	The Nicotinic Agonist Cytisine: The Role of the NH ₂ -N Interaction. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 9991-9996.	2.1	1
13116	Predicting DNA-Reactivity of N-Nitrosamines: A Quantum Chemical Approach. <i>Chemical Research in Toxicology</i> , 2022, 35, 2068-2084.	1.7	10
13117	Predicting band gaps and band-edge positions of oxide perovskites using density functional theory and machine learning. <i>Physical Review B</i> , 2022, 106, .	1.1	4
13118	Non-empirical double-hybrid density functionals as reliable tools for electronic structure calculations. <i>Electronic Structure</i> , 2022, 4, 043001.	1.0	4
13119	A Thermally Activated Delayed Fluorescence Emitter Investigated by Time-Resolved Near-Infrared Spectroscopy. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	4
13120	Density functional theory demonstrates orientation effects in the Raman spectra of hydroxy- and carbonated apatite. <i>Journal of Raman Spectroscopy</i> , 2023, 54, 159-170.	1.2	1
13121	Impacts of polarizable continuum models on the SCF convergence and DFT delocalization error of large molecules. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	2
13122	PtO _x Cl _y (OH) _z (H ₂ O) _n Complexes under Oxidative and Reductive Conditions: Impact of the Level of Theory on Thermodynamic Stabilities. <i>ChemPhysChem</i> , 2023, 24, .	1.0	3
13123	Effects of additional ĩ-spacers on the photovoltaic properties of organic dyes for efficient dye-sensitized solar cells: a theoretical study. <i>Research on Chemical Intermediates</i> , 2022, 48, 5243-5264.	1.3	1
13124	Computational design of magnetic molecules and their environment using quantum chemistry, machine learning and multiscale simulations. <i>Nature Reviews Chemistry</i> , 2022, 6, 761-781.	13.8	21
13125	In Situ Kinetic Studies of Rh(II)-Catalyzed C-H Functionalization to Achieve High Catalyst Turnover Numbers. <i>ACS Catalysis</i> , 2022, 12, 13400-13410.	5.5	6
13126	Nano-crystalline precursor formation, stability, and transformation to mullite-type visible-light photocatalysts. <i>Journal of Materials Science</i> , 2022, 57, 19280-19299.	1.7	3
13127	QM/MM Study of Partial Dissociation of S2B for the E ₂ Intermediate of Nitrogenase. <i>Inorganic Chemistry</i> , 2022, 61, 18067-18076.	1.9	7
13128	Anticoagulants as Potential SARS-CoV-2 Mpro Inhibitors for COVID-19 Patients: In Vitro, Molecular Docking, Molecular Dynamics, DFT, and SAR Studies. <i>International Journal of Molecular Sciences</i> , 2022, 23, 12235.	1.8	18
13129			

#	ARTICLE	IF	CITATIONS
13133	Electronic structure of curcuminoids with potential medicinal applications: a theoretical insight. <i>Structural Chemistry</i> , 2023, 34, 1427-1438.	1.0	1
13134	New Theoretical Insights about Anticorrosive Effects and Adsorption Mechanism of Some $\hat{\pm}$ -Amino Acids on Al Surface: DFT, MEP, FMO, NBO, QSAR, Fukui Functions and Monte Carlo Simulation. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2022, 58, 1054-1070.	0.3	3
13135	DFT calculations of ^1H - and ^{13}C -NMR chemical shifts of 3-methyl-1-phenyl-4-(phenyldiazenyl)-1H-pyrazol-5-amine in solution. <i>Scientific Reports</i> , 2022, 12, .	1.6	9
13136	Electrochemical Strategy for Proton Relay Installation Enhances the Activity of a Hydrogen Evolution Electrocatalyst. <i>Journal of the American Chemical Society</i> , 2022, 144, 20267-20277.	6.6	8
13137	Turn Off "On Fluorescent CO_2 Gas Detection Based on Amine-Functionalized Imidazole-Based Poly(ionic liquid). <i>ACS Omega</i> , 2022, 7, 40485-40492.	1.6	3
13138	Extremely Suppressed Energetic Disorder in a Chemically Doped Conjugated Polymer. <i>Advanced Materials</i> , 2023, 35, .	11.1	5
13139	Benchmarking Density Functionals, Basis Sets, and Solvent Models in Predicting Thermodynamic Hydricities of Organic Hydrides. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7566-7577.	1.1	0
13140	Effect of the Silica "Magnetite Nanocomposite Coating Functionalization on the Doxorubicin Sorption/Desorption. <i>Pharmaceutics</i> , 2022, 14, 2271.	2.0	7
13141	When Gold Is Not Enough: Platinum Standard of Quantum Chemistry with $\langle i \rangle \text{N} \langle i \rangle^{\langle \sup \rangle 7} \langle /sup \rangle$ Cost. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 6537-6556.	2.3	5
13142	Key Selectivity Controlling Elements in Rhodium-Catalyzed C-H Functionalization with Donor/Acceptor Carbenes. <i>ACS Catalysis</i> , 2022, 12, 13446-13456.	5.5	6
13143	Theoretical investigation by DFT and TDDFT the extension of π -conjugation of novel carbazole-based donor materials for bulk heterojunction organic solar cell applications. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	3
13144	Modeling Charge Transfer Reactions by Hopping between Electronic Ground State Minima: Application to Hole Transfer between DNA Bases. <i>Molecules</i> , 2022, 27, 7408.	1.7	3
13145	Hydrogen Bonding in Platinum Indolylphosphine Polyfluorido and Fluorido Complexes. <i>Chemistry - A European Journal</i> , 0, , .	1.7	3
13146	Facile synthesis and photodetection characteristics of new pyrrolo[2,3-b]pyrrole-based metal-free organic dyes containing phenols as the potential candidates towards energy conversion. <i>Materials Chemistry and Physics</i> , 2023, 293, 126972.	2.0	7
13147	Structure and stability of MCl_4 carbene complexes ($\text{M} = \text{Si}, \text{Ge}, \text{Sn}$): Experiment and theory. <i>Journal of Organometallic Chemistry</i> , 2023, 983, 122551.	0.8	2
13148	Structural, electronic and optical properties of the wide band gap semiconductors KGaQ_2 ($\text{Q} = \text{S}, \text{Se}$) and of AGaTe_2 ($\text{A} = \text{K}, \text{Cs}$). <i>Revista Mexicana De Física</i> , 2022, 68, .	0.2	0
13149	Insights of hydrogen adsorption and dissociation on Ni doped Mg_4 clusters: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113907.	1.1	5
13150	Importance of amine in carbon dioxide conversion to methanol catalyzed by Ru-PNP complex. <i>Molecular Catalysis</i> , 2022, 532, 112729.	1.0	1

#	ARTICLE	IF	CITATIONS
13151	Reliable gas-phase tautomer equilibria of drug-like molecule scaffolds and the issue of continuum solvation. <i>Journal of Computer-Aided Molecular Design</i> , 0, , .	1.3	4
13152	First-principles study of the structural and electronic properties of BN-ring doped graphene. <i>Physical Review Materials</i> , 2022, 6, .	0.9	1
13154	Revealing the Unexplored Mechanism of Photochemical Oxaziridine Conversion Process of 2H-imidazole 1-oxides. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0
13155	Comparative analyses and molecular videography of MD simulations on WT human SOD1. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113929.	1.1	0
13156	Nickel-Catalyzed Radical Heck-Type C(sp ³)-C(sp ²) Coupling Cascades Enabled by Bromoalkane-Directed 1,4-Aryl Shift: Access to Olefinated Arylalanines. <i>Organic Letters</i> , 2022, 24, 8192-8196.	2.4	3
13157	B3Al4+: A Three-Dimensional Molecular Reuleaux Triangle. <i>Molecules</i> , 2022, 27, 7407.	1.7	4
13158	Kinetics of the R ² O ₂ 'R ² HO+OH reactions of substituted methyl radicals: Effects of Cl, F, and CF ₃ substitution and notes on the RO+O producing channel. <i>Chemical Physics Letters</i> , 2022, 808, 140121.	1.2	1
13159	Difference in the hydration state of water at the hydrophobic interface of structural isomers of propanol investigated by U.V visible absorption and Raman spectroscopic study. <i>Journal of Molecular Liquids</i> , 2022, 368, 120530.	2.3	1
13160	Experimental and theoretical studies of photophysical properties of N-Substituted iminocoumarins. <i>Optical Materials</i> , 2022, 134, 113113.	1.7	1
13161	Unexpected formation of 2-methyl-1H-naphtho [2, 3-d] imidazole via decarboxylation governed mechanistic pathway. <i>Chemical Physics</i> , 2023, 565, 111735.	0.9	0
13162	Carbazole based D-π-A dyes for DSSC applications: DFT/TDDFT study of the influence of π-spacers on the photovoltaic performance. <i>Chemical Physics</i> , 2023, 565, 111738.	0.9	5
13163	A theoretical investigation of the possible mechanisms for detection the copper ions by a retinal-base sensor. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 436, 114363.	2.0	1
13164	Spectroscopic, crystal structure, antimicrobial and antioxidant evaluations of new Schiff base compounds: An experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2023, 1273, 134382.	1.8	10
13165	Design, synthesis, characterization, antioxidant, antiproliferative activity and molecular docking studies of new transition metal complexes of 1,2,4-triazole as combretastatin A-4 analogues. <i>Journal of Molecular Structure</i> , 2023, 1274, 134437.	1.8	1
13166	A comparative study on photophysics of meso-substituted mono- and bis-BODIPY carbazoles. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 436, 114356.	2.0	4
13167	Asian Ancistrocladus Lianas as Creative Producers of Naphthylisoquinoline Alkaloids. <i>Progress in the Chemistry of Organic Natural Products</i> , 2023, , 1-335.	0.8	3
13168	The organic co-crystals formed using naphthalenediimide-based triangular macrocycles and coronene: intermolecular charge transfers and nonlinear optical properties. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 29747-29756.	1.3	5
13169	Theoretical exploration of molecular packing and the charge transfer mechanism of organic solar cells based on PM6:Y6. <i>Journal of Materials Chemistry A</i> , 2022, 10, 25611-25619.	5.2	6

#	ARTICLE	IF	CITATIONS
13170	<i>cis</i> → <i>trans</i> isomerization of dimethyl 2,3-dibromofumarate. <i>RSC Advances</i> , 2022, 12, 32471-32474.	1.7	0
13171	Uniaxial strain tuning of organic molecule single photon sources. <i>Nanoscale</i> , 2022, 15, 177-184.	2.8	1
13172	Hidden Intermediate Activation: A Concept to Elucidate the Reaction Mechanism of the Schmittel Cyclization of Enyne-Allenenes. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	4
13173	A Photo-Basic D-A Fluorophore with a High Intramolecular Charge-Transfer as Model Strategy for Designing Organic Proton-Coupled Electron-Transfer Modulators: An Analysis based on Steady-State Fluorescence, Isotopic Effect and Theoretical Study. <i>Molecular Systems Design and Engineering</i> , 0, , .	1.7	2
13174	Eco-friendly Enteromorpha polysaccharides-based hydrogels for heavy metal adsorption: From waste to efficient materials. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 656, 130531.	2.3	14
13175	Investigation of kinetics and mechanistic insights of the reaction of criegee intermediate (CH ₂ OO) with methyl-ethyl ketone (MEK) under tropospherically relevant conditions. <i>Chemosphere</i> , 2023, 312, 137217.	4.2	3
13176	A novel pH-Dependent sensor for recognition of strontium ions in water: A hierarchically structured mesoporous architectonics. <i>Talanta</i> , 2023, 253, 124064.	2.9	1
13177	D-D- <i>A</i> - <i>A</i> -based quinoxaline dyes incorporating phenothiazine, phenoxazine and carbazole as electron donors: Synthesis, photophysical, electrochemical, and computational investigation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 436, 114389.	2.0	8
13178	Investigation and design of efficient intramolecular charge transfer dyes with DBTP-based dual-electron-donor structure. <i>Materials Science in Semiconductor Processing</i> , 2023, 154, 107203.	1.9	0
13179	Quantum Chemical Benchmark Study on Valdecoxib, a Potent and Selective Inhibitor of COX-2, and its Hydroxylated Derivative. <i>Cumhuriyet Science Journal</i> , 2022, 43, 221-231.	0.1	1
13180	First-principles redox energy estimates under the condition of satisfying the general form of Koopmans's theorem: An atomistic study of aqueous iron. <i>Journal of Chemical Physics</i> , 2022, 157, 184110.	1.2	0
13182	One-Bond ¹³ C→ ¹ H and ¹³ C→ ¹³ C Spin-Coupling Constants as Constraints in <i>MAAT</i> Analysis of Saccharide Conformation. <i>Journal of Physical Chemistry B</i> , 2022, 126, 9506-9515.	1.2	4
13183	Theoretical investigation of structural parameters, reactivity behavior, and thermodynamic properties of Anderson polyoxometalate (POM). <i>Structural Chemistry</i> , 2023, 34, 1231-1240.	1.0	4
13184	Evaluation of Crocin as green corrosion inhibitor for aluminum in NaCl solution. <i>Chemical Engineering Communications</i> , 0, , 1-17.	1.5	0
13185	Computational investigation on mechanisms and kinetics of gas-phase reactions of 4-hydroxy-2-pentanone (4H2P) with hydroxyl radicals and subsequent reactions of CH ₃ C(O)CH ₂ ·(OH)CH ₃ radical. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	0
13186	Unlocking cell chemistry evolution with operando fibre optic infrared spectroscopy in commercial Na(Li)-ion batteries. <i>Nature Energy</i> , 2022, 7, 1157-1169.	19.8	35
13187	Thermochemistry of perfluoroalkyl and polyfluoroalkyl substances. <i>Journal of Computational Chemistry</i> , 2023, 44, 570-580.	1.5	4
13188	Synthesis, characterization and computational investigation of the phosphatase activity of a dinuclear Zinc(II) complex containing a new heptadentate asymmetric ligand. <i>Journal of Inorganic Biochemistry</i> , 2022, , 112064.	1.5	1

#	ARTICLE	IF	CITATIONS
13189	Extended π -Conjugated Ligands Tune Excited-State Energies of Iron(II) Polypyridine Dyes. <i>Inorganic Chemistry</i> , 2022, 61, 18850-18860.	1.9	2
13190	Spectroscopic, structural and computational studies of thiophenolato bridged dirhenium(III,III) complexes. <i>Journal of Coordination Chemistry</i> , 2022, 75, 2829-2842.	0.8	1
13191	Absorption Spectra of Flexible Fluorescent Probes by a Combined Computational Approach: Molecular Dynamics Simulations and Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8809-8817.	1.1	2
13192	Electronic and photophysical properties of selected organic boron-containing molecules: Insight into effects of heteroatom substitution and aggregation. <i>Journal of the Chinese Chemical Society</i> , 0, , .	0.8	0
13193	Variable Kinetic Isotope Effect Reveals a Multistep Pathway for Protonolysis of a Pt ^{II} -Me Bond. <i>Organometallics</i> , 2022, 41, 3770-3780.	1.1	1
13194	Synthesis, characterization, and quantum chemical study of cobalt(II) chelates with <i>N</i> -phenethyl-iminodiacetate(2-)-like ligands. Influence of <i>p</i> -(<i>R</i>)-phenethyl group on crystal pattern. <i>Journal of Coordination Chemistry</i> , 2022, 75, 2814-2828.	0.8	1
13195	Strategies to Enhance the Rate of Proton-Coupled Electron Transfer Reactions in Dye-Water Oxidation Catalyst Complexes. <i>ChemPhotoChem</i> , 0, , .	1.5	0
13196	Effects of chelate ligands containing NN, PN, and PP on the performance of half-sandwich ruthenium metal complexes as sensitizers in dye sensitized solar cells (DSSCs): Quantum chemical investigation. <i>Polyhedron</i> , 2023, 230, 116190.	1.0	3
13197	Kinetic and Mechanistic Study of the Reactions of NO ₃ Radicals with Unsaturated Aldehydes: 2-Butenal, 2-Methyl-2-butenal, and 3-Methyl-2-butenal. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8682-8694.	1.1	1
13198	In vitro cytotoxicity activity of copper complexes of imine and amine ligands: A combined experimental and computational study. <i>Inorganic Chemistry Communication</i> , 2022, 146, 110190.	1.8	2
13199	Sustainable and efficient recovery of lithium from sodium sulfate by-product of lithium hydroxide production process using solvent extraction. <i>Minerals Engineering</i> , 2022, 190, 107907.	1.8	3
13200	Theoretical investigation of the Zn ²⁺ detection mechanism based on the quinoline derivative of the Schiff-base receptor. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 287, 122123.	2.0	5
13201	Molecular investigation of interplay mechanism between polydopamine and graphene oxide: The effect of oxidation degree on the adsorption behavior of polydopamine. <i>Applied Surface Science</i> , 2023, 611, 155759.	3.1	6
13202	Redshifted and thermally bistable one-way quantitative hemithioindigo-derived photoswitches enabled by isomer-specific excited state intramolecular proton transfer. <i>Chemical Communications</i> , 2023, 59, 563-566.	2.2	5
13203	XDM-corrected hybrid DFT with numerical atomic orbitals predicts molecular crystal lattice energies with unprecedented accuracy. <i>Chemical Science</i> , 2023, 14, 1252-1262.	3.7	14
13204	Ethyl ester/acyl hydrazide-based aromatic sulfonamides: facile synthesis, structural characterization, electrochemical measurements and theoretical studies as effective corrosion inhibitors for mild steel in 1.0 M HCl. <i>RSC Advances</i> , 2022, 13, 186-211.	1.7	11
13205	Effect of electronic structure of energy transfer in bimetallic Ru(ⁱⁱ)/Os(ⁱⁱ) complexes. <i>Dalton Transactions</i> , 2023, 52, 990-999.	1.6	2
13206	Topology of the Electronic Current Density Induced by a Static Magnetic Field in Lithium Hydride, Water, Ammonia and Methane Molecules. , 2024, , 175-188.		0

#	ARTICLE	IF	CITATIONS
13207	A quantum chemical analysis of an organic compound: 3,5-bis (4-hydroxy phenyl)-2,4,6-trimethyl cyclohexanone. AIP Conference Proceedings, 2022, , .	0.3	2
13208	The eight structures of caffeic acid: a jet-cooled laser ablated rotational study. RSC Advances, 2022, 13, 212-219.	1.7	0
13209	Competitive adsorption of anionic and cationic molecules on three activated carbons derived from agroindustrial waste. Biomass and Bioenergy, 2023, 168, 106660.	2.9	8
13210	Theoretical investigations of positron affinities and their structure-dependent properties of carbon dioxide clusters (CO ₂) _n (<i>n</i> = 1–5). Physical Chemistry Chemical Physics, 2022, 25, 625-632.	1.3	1
13211	An ultra-thin polymer electrolyte for 4.5 ÅV high voltage LiCoO ₂ quasi-solid-state battery. Chemical Engineering Journal, 2023, 455, 140846.	6.6	11
13212	Carbazole-substituted benzobisoxazoles: near-UV fluorescent emitters and ambipolar hosts for organic light-emitting diodes. Journal of Materials Chemistry C, 2022, 11, 211-222.	2.7	2
13213	Rhodium-catalyzed enantioselective C–H alkynylation of sulfoxides in diverse patterns: desymmetrization, kinetic resolution, and parallel kinetic resolution. Chemical Science, 2023, 14, 317-322.	3.7	4
13214	New charge-transfer complexes of 1,2,5-chalcogenadiazoles with tetrathiafulvalenes. CrystEngComm, 2023, 25, 391-402.	1.3	3
13215	First-principles studies of the caged germanium clusters with gold doping and their adsorption on graphdiyne nanosheets. Journal of Molecular Liquids, 2023, 370, 120968.	2.3	2
13216	Engineering aluminosilicate's photochromism by quantum chemistry. Journal of Materials Chemistry C, 2023, 11, 730-741.	2.7	2
13217	Phenylethynylantracene based push–pull molecular systems: tuning the photophysics through <i>para</i> -substituents on the phenyl ring. Physical Chemistry Chemical Physics, 0, , .	1.3	0
13218	Search for stable host materials as low-voltage anodes for lithium-ion batteries: A mini-review. Energy Storage Materials, 2023, 55, 364-387.	9.5	11
13219	A comprehensive benchmark investigation of quantum chemical methods for carbocations. Physical Chemistry Chemical Physics, 2023, 25, 1903-1922.	1.3	3
13220	Modelling single atom catalysts for water splitting and fuel cells: A tutorial review. Journal of Power Sources, 2023, 556, 232492.	4.0	19
13221	Density functional theory study of the sensing of ozone gas molecules by using fullerene-like Group-III nitride nanostructures. Physica B: Condensed Matter, 2023, 650, 414553.	1.3	6
13222	Substituted naphthoxy-phthalonitrile derivatives: Synthesis, substituent effects, DFT, TD-DFT Calculations, antimicrobial properties and DNA interaction studies. Computational Biology and Chemistry, 2023, 102, 107798.	1.1	4
13223	Flexible, graphene protected Ag nanoparticles–polyimide tape for use as a transparent Surface-Enhanced Raman Scattering (SERS) substrate and its application in pesticide detection. Nano Structures Nano Objects, 2023, 33, 100930.	1.9	3
13224	The catalytic performance enhanced via π -electron cloud interaction of polymerized cobalt phthalocyanine/3D-graphene as bifunctional oxygen catalysts for Zn-air battery. Journal of Power Sources, 2023, 556, 232471.	4.0	7

#	ARTICLE	IF	CITATIONS
13225	Research on the hydrothermal regeneration of powdered activated coke in wastewater treatment. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109120.	3.3	4
13226	Multiscale calculation of carrier mobility in organic solids through the fine-tuned kinetic Monte Carlo simulation. <i>Computational Materials Science</i> , 2023, 218, 111957.	1.4	0
13227	Experimental and theoretical study on the regioselective bis- or polyalkylation of 6-amino-2-mercapto-3 <i>H</i> -pyrimidin-4-one using zeolite nano-gold catalyst and a quantum hybrid computational method. <i>RSC Advances</i> , 2022, 12, 35794-35808.	1.7	2
13228	Decomposition analysis on the excitation behaviors of thiazolothiazole (TTz)-based dyes <i>via</i> the time-dependent dielectric density functional theory approach. <i>RSC Advances</i> , 2022, 12, 34685-34693.	1.7	3
13229	Formation of a Resonance-Stabilized Radical Intermediate by Hydroxyl Radical Addition to Cyclopentadiene. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9031-9041.	1.1	0
13230	Separation of Radioactive Ruthenium from Alkaline Solution: A Solvent Extraction and Detailed Mechanistic Approach. <i>ACS Omega</i> , 2022, 7, 43803-43812.	1.6	1
13231	Computational Study of a Novel Compound with Thioether-Bridge. <i>Polycyclic Aromatic Compounds</i> , 0, 1-21.	1.4	0
13232	Pyrazole Derivative Containing Naphthalene Moiety: Cytotoxicity (Breast and Cervical Cancer), Antibacterial and Antifungal Studies Using Experimental and Theoretical Tools. <i>Polycyclic Aromatic Compounds</i> , 0, 1-18.	1.4	0
13233	Trapping the Transition State in a [2,3]-Sigmatropic Rearrangement by Applying Pressure. <i>ACS Omega</i> , 2022, 7, 45208-45214.	1.6	3
13234	Nonfullerene Acceptors Based on Naphthalene Substituted Thieno[3,2- <i>b</i>]thiophene Core for Efficient Organic Solar Cells. <i>Russian Journal of General Chemistry</i> , 2022, 92, 2354-2362.	0.3	0
13235	Molecular Dynamics Simulation of the Thermal Behavior of Hydroxyapatite. <i>Nanomaterials</i> , 2022, 12, 4244.	1.9	4
13236	Not All ³ MC States Are the Same: The Role of ³ MC _{cis} States in the Photochemical N ³ S ⁺ N Ligand Release from [Ru(bpy) ₂ (N ³ S ⁺ N)] ²⁺ Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 19907-19924.	1.9	8
13237	Pressure-assisted decomposition of tricresyl phosphate on amorphous <i>FeO</i> using hybrid quantum-classical simulations. <i>Journal of Computational Chemistry</i> , 2023, 44, 766-776.	1.5	2
13238	Designing metal chelates of halogenated sulfonamide Schiff bases as potent nonplatinum anticancer drugs using spectroscopic, molecular docking and biological studies. <i>Scientific Reports</i> , 2022, 12, .	1.6	5
13239	Novel Carbonyl Cathode for Green and Sustainable Aluminum Organic Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 53702-53710.	4.0	13
13240	Two Theorems and Important Insight on How the Preferred Mechanism of Free Radical Scavenging Cannot Be Settled. Comment on Pandithavidana, D.R.; Jayawardana, S.B. Comparative Study of Antioxidant Potential of Selected Dietary Vitamins; <i>Computational Insights. Molecules</i> 2019, 24, 1646. <i>Molecules</i> , 2022, 27, 8092.	1.7	4
13241	Development of QSRR model for hydroxamic acids using PCA-GA-BP algorithm incorporated with molecular interaction-based features. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	2
13242	Testing of Exchange-Correlation Functionals of DFT for a Reliable Description of the Electron Density Distribution in Organic Molecules. <i>International Journal of Molecular Sciences</i> , 2022, 23, 14719.	1.8	7

#	ARTICLE	IF	CITATIONS
13243	Computational Screening of D- π -A Structured with Acceptor Tuned Metal-Free Organic Dye Molecules for DSSCs. <i>Journal of Computational Biophysics and Chemistry</i> , 0, , .	1.0	1
13244	Femtosecond Spectroscopy and Quantum Chemistry of a Linearly Coordinated Copper(I) Carbene Complex. <i>ChemPhotoChem</i> , 2023, 7, .	1.5	2
13246	C ₃ -symmetric tripalladium(II) complex for catalysis via geometrical coincident interaction with C ₃ -symmetric substrate. <i>Transition Metal Chemistry</i> , 0, , .	0.7	0
13247	Solvent-Induced Spin-State Change in Copper Corroles. <i>Inorganic Chemistry</i> , 2022, 61, 20288-20298.	1.9	4
13248	Crystal Structure of <i>N</i> -(2-Hydroxynaphthylidene)- <i>L</i> -isoleucinyl-4,6-dimethylidene- β -D-glucopyranosylamine and an Insight from Experimental and Theoretical Calculations. <i>Crystal Research and Technology</i> , 0, , 2200209.	0.6	2
13249	$\langle \text{mml:msup} \langle \text{mml:mi mathvariant="normal"} \rangle \text{coronene} \langle \text{mml:mo} \rangle + \langle \text{mml:mo} \rangle \langle \text{mml:msup} \rangle \langle \text{mml:math} \rangle$ and $\langle \text{mml:math} \rangle$ xmlns:mml="http://www.w3.org/1998/Math/MathML" > $\langle \text{mml:msup} \langle \text{mml:mrow} \langle \text{mml:mo} \rangle \langle \text{mml:mo} \rangle \langle \text{mml:mtext} \rangle \text{coronene} \langle \text{mml:mo} \rangle \langle \text{mml:msup} \rangle \langle \text{mml:math} \rangle$	1.0	2
13250	On the Cooperative Origin of Solvent-Enhanced Symmetry-Breaking Charge Transfer in a Covalently Bound Tetracene Dimer Leading to Singlet Fission. <i>Journal of the American Chemical Society</i> , 2022, 144, 23492-23504.	6.6	7
13251	Modeling the electronic structure of organic materials: a solid-state physicist's perspective. <i>JPhys Materials</i> , 2023, 6, 012001.	1.8	8
13252	Three- and Five-membered Anionic Chains of Pnictogenylboranes. <i>Chemistry - A European Journal</i> , 0, , .	1.7	1
13253	Studies on the Efficiency of Iron Release from Fe(III)-EDTA and Fe(III)-Cit and the Suitability of These Compounds for Tetracycline Degradation. <i>Molecules</i> , 2022, 27, 8498.	1.7	2
13254	Ag(III)- π -Ag(III) Argentophilic Interaction in a Cofacial Corrole Dyad. <i>Inorganic Chemistry</i> , 2023, 62, 3-17.	1.9	3
13255	Intersystem Crossing and Intramolecular Triplet Excitation Energy Transfer in Spiro[9,10-dihydro-9-oxoanthracene-10,2'-5,6'-benzindan] Investigated by DFT/MRCI Methods. <i>Canadian Journal of Chemistry</i> , 0, , .	0.6	0
13256	TM ₂ -B ₂ Quadruple Active Sites Supported on a Defective C ₃ N Monolayer as Catalyst for the Electrochemical CO ₂ Reduction: A Theoretical Perspective. <i>ChemSusChem</i> , 2023, 16, .	3.6	3
13257	Evolving the complexities of glycine magnesium chloride (GMC) crystal through DFT computation for NLO utilizations. <i>Journal of Molecular Structure</i> , 2023, 1277, 134839.	1.8	1
13258	In Quest of Low-Leakage Dynamic Random Access Memory Enabled by Doped TiO ₂ Dielectrics. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	1
13259	Insight into the Alkaline Stability of Arylene-Linked Bis-Benzimidazoles and Polybenzimidazoles. <i>ACS Applied Polymer Materials</i> , 2023, 5, 803-814.	2.0	8
13260	Strychnos alkaloids: total synthesis, characterization, DFT investigations, and molecular docking with AChE, BuChE, and HSA. <i>Heliyon</i> , 2022, 8, e11990.	1.4	3
13261	All Visible Light Photoswitch Based on the Dimethyldihydropyrene Unit Operating in Aqueous Solutions with High Quantum Yields. <i>Jacs Au</i> , 2023, 3, 131-142.	3.6	7

#	ARTICLE	IF	CITATIONS
13262	Introduction to Electrocatalysts. ACS Symposium Series, 0, , 1-37.	0.5	6
13263	Self Cycloaddition of <i>o</i> -Naphthoquinone Nitrosomethide to (Å±) Spiro{naphthalene(naphthopyranofurazan)}one Oxide: An Insight into its Formation. ChemPlusChem, 2022, 87, .	1.3	2
13264	Mechanistic Details of the Pd-catalyzed and MPAA Ligand-Enabled $\text{I}^2\text{A}(\text{sp}^3)\text{H}$ Acetoxylation of Free Carboxylic Acid. Chemistry - an Asian Journal, 0, , .	1.7	0
13265	Fully Tin-Coated Coinage Metal Ions: A Pincer-Type Bis-stannylene Ligand for Exclusive Tetrahedral Complexation. Chemistry - A European Journal, 2023, 29, .	1.7	6
13266	Building on the strengths of a double-hybrid density functional for excitation energies and inverted singlet-triplet energy gaps. Journal of Chemical Physics, 2023, 158, .	1.2	3
13267	The effect of alkali metals, carbocations, and metallocenes substitutes on two $\text{I}^{1/2}$ -carrabiose disaccharide derivatives: a density functional study. Structural Chemistry, 0, , .	1.0	0
13268	Copper(II) chelates derived from an N,N,O-tridentate 2-pyridinecarboxaldehyde-N4-phenylsemicarbazone: Synthesis, spectral aspects, crystal structure, FMO and NBO analysis. Journal of Molecular Structure, 2023, 1277, 134866.	1.8	4
13269	ESIPT-active cinnamoyl pyrones are bright solid-state emitters: Revisited theoretical approach and experimental study. Dyes and Pigments, 2023, 211, 111046.	2.0	6
13270	Cu(I)/Cu(II) Creutz-Taube Mixed-Valence 2D Coordination Polymers. Small Methods, 0, , 2201166.	4.6	1
13271	Optoelectronic design and charge transport properties of Benzodifuran (BDF) isomers for organic electronic devices: DFT/TD-DFT insights. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2023, 290, 122266.	2.0	10
13272	Mind the Interface Gap: Exposing Hidden Interface Defects at the Epitaxial Heterostructure between CuO and Cu_2O . ACS Applied Materials & Interfaces, 2022, 14, 56331-56343.	4.0	1
13273	Contradictory Role of Locally-Excited Triplet States in Blue Thermally Activated Delayed Fluorescence of <i>s</i> -Triazine-Based Emitters. Journal of Physical Chemistry C, 2023, 127, 358-367.	1.5	1
13274	DeePKS + ABACUS as a Bridge between Expensive Quantum Mechanical Models and Machine Learning Potentials. Journal of Physical Chemistry A, 2022, 126, 9154-9164.	1.1	4
13275	Samarium Diiodide Acting on Acetone Modeling Single Electron Transfer Energetics in Solution. Molecules, 2022, 27, 8673.	1.7	0
13276	Development of Nonlocal Kinetic-Energy Density Functional for the Hybrid QM/MM Interaction. Journal of Chemical Physics, 0, , .	1.2	2
13277	Finding Design Principles of OLED Emitters through Theoretical Investigations of Zn(II) Carbene Complexes. Inorganic Chemistry, 2022, 61, 20896-20905.	1.9	2
13278	Gas-Phase Formation of 1,3,5,7-Cyclooctatetraene (C_8H_8) through Ring Expansion via the Aromatic 1,3,5-Cyclooctatrien-7-yl Radical (C_8H_9^+) Transient. Journal of the American Chemical Society, 2022, 144, 22470-22478.	6.6	1
13279	TDDFT versus <i>GW</i> /BSE Methods for Prediction of Light Absorption and Emission in a TADF Emitter. Journal of Physical Chemistry A, 2022, 126, 9627-9643.	1.1	1

#	ARTICLE	IF	CITATIONS
13280	Structural Investigation of DHICA Eumelanin Using Density Functional Theory and Classical Molecular Dynamics Simulations. <i>Molecules</i> , 2022, 27, 8417.	1.7	0
13281	Interexcited State Photophysics I: Benchmarking Density Functionals for Computing Nonadiabatic Couplings and Internal Conversion Rate Constants. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 271-292.	2.3	5
13282	Differential gene expression analysis of RAGE-100A6 complex for target selection and the design of novel inhibitors for anticancer drug discovery. <i>Journal of Cellular Biochemistry</i> , 2023, 124, 205-220.	1.2	3
13283	<i>In-Silico</i> Partial N ₂ to NH ₃ Conversion with a Light Atom Molecule. <i>ChemPhysChem</i> , 2023, 24, .	1.0	1
13284	Reactions of Thorium Oxide Clusters with Water: the Effects of Oxygen Content. <i>ChemPhysChem</i> , 0, , .	1.0	0
13285	Synthesis and Antitrypanosomal and Mechanistic Studies of a Series of 2-Arylquinazolin-4-hydrazines: A Hydrazine Moiety as a Selective, Safe, and Specific Pharmacophore to Design Antitrypanosomal Agents Targeting NO Release. <i>ACS Omega</i> , 2022, 7, 47225-47238.	1.6	4
13286	Electronic Structure and Magnetic Properties of a High-Spin Mn ^{III} Complex: [Mn(mesacac) ₃] (mesacac=1,3-Bis(2,4,6-trimethylphenyl)propane-1,3-dionato). <i>ChemPhysChem</i> , 0, , .	1.0	1
13287	Attachment Chemistry of 4-Fluorophenylboronic Acid on TiO ₂ and Al ₂ O ₃ Nanoparticles. <i>Chemistry of Materials</i> , 2022, 34, 10659-10669.	3.2	2
13288	High-Throughput Computational Screening of Two-Dimensional Semiconductors. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 11581-11594.	2.1	51
13289	Synthesis and Crystal Structure of Adamantylated 4,5,6,7-Tetrahalogeno-1H-benzimidazoles Novel Multi-Target Ligands (Potential CK2, M2 and SARS-CoV-2 Inhibitors); X-ray/DFT/QTAIM/Hirshfeld Surfaces/Molecular Docking Study. <i>Molecules</i> , 2023, 28, 147.	1.7	3
13290	Spintronic action of C _n -C ₆ H ₆ -Fe-C ₆ H ₆ -C ₁₃ -n; n = 6: How crucial are d electrons?. <i>Journal of Molecular Structure</i> , 2023, 1277, 134836.	1.8	0
13291	Evaluations of molecular modeling and machine learning for predictive capabilities in binding of lanthanum and actinium with carboxylic acids. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 0, , .	0.7	0
13292	Computational Study of Iron-Catalyzed Intramolecular [2 + 2] Cycloaddition and Cycloisomerization of Enyne Acetates: Mechanism and Selectivity. <i>Journal of Organic Chemistry</i> , 2023, 88, 944-951.	1.7	0
13293	Vibrationally resolved two-photon electronic spectra including vibrational pre-excitation: Theory and application to VIPER spectroscopy with two-photon excitation. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	1
13294	Synthesis, crystal structure, DFT, Hirshfeld surface analysis, energy framework, docking and molecular dynamic simulations of (E)-4-(4-methylbenzyl)-6-styrylpyridazin-3(2H)-one as anticancer agent. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 11578-11597.	2.0	4
13295	Bond breaking of furan-maleimide adducts via a diradical sequential mechanism under an external mechanical force. <i>Chemical Science</i> , 2023, 14, 1263-1271.	3.7	3
13296	Synthesis, Structural, Magnetic and Computational Studies of a One-Dimensional Ferromagnetic Cu(II) Chain Assembled from a New Schiff Base Ligand. <i>Chemistry</i> , 2023, 5, 85-96.	0.9	0
13297	An Air- and Moisture-Stable Zinc(II) Carbene Dithiolate Dimer Showing Fast Thermally Activated Delayed Fluorescence and Dexter Energy Transfer Catalysis**. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	6

#	ARTICLE	IF	CITATIONS
13298	Advancing Electrode Properties through Functionalization for Solid Oxide Cells Application: A Review. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	3
13299	Ionization energies of metallocenes: A coupled cluster study of cobaltocene. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	3
13300	Design, synthesis, molecular modelling and antitumor evaluation of <i>S</i> -glucosylated rhodanines through topo II inhibition and DNA intercalation. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2023, 38, .	2.5	2
13301	DFT computations combined with semiempirical modeling of variations with temperature of spectroscopic and magnetic properties of Gd ³⁺ -doped PbTiO ₃ . <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
13302	Possible Role of Metal-Ions in the Chemistry of Prochirality and the Origin of Chirality in the Interstellar Medium. <i>ACS Earth and Space Chemistry</i> , 2023, 7, 77-91.	1.2	1
13303	Dinitrogen reduction using ruthenium coordinated by nitrogen-doped graphene and cobalt complex coordinated by anionic PNP pincer ligand as catalysts and Frustrated Lewis Pair as a co-catalyst: Density Functional Theory studies. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	2
13304	The structure of the high-affinity nickel-binding site in the Ni ₂ Zn-HypA-UreE2 complex. <i>Metallomics</i> , 2023, 15, .	1.0	4
13305	Observation of slow magnetic relaxation phenomena in spatially isolated π -radical ions. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1
13306	Homo-valent diruthenium(μ_2 , μ_2) carbonates Na ₄ [Ru ₂ (CO ₃) ₄] \cdot 10H ₂ O: synthesis, structure, properties, and calculation. <i>Dalton Transactions</i> , 0, , .	1.6	1
13307	Relativistic Effects from Heavy Main Group p-Elements on the NMR Chemical Shifts of Light Atoms: From Pioneering Studies to Recent Advances. <i>Magnetochemistry</i> , 2023, 9, 24.	1.0	9
13308	Metal-Free Catalytic Functionalization of Second π -C _{sp} ² π -H Bond of 1-Methyl Pyrrole Using Bishomocubane-Derived Aminoborane Frustrated Lewis Pairs: A Computational Study. <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
13309	Full Implementation, Optimization, and Evaluation of a Range-Separated Local Hybrid Functional with Wide Accuracy for Ground and Excited States. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 488-502.	2.3	14
13310	Site-Selective Atomic Layer Deposition on Rutile TiO ₂ : Selective Hydration as a Route to Target Point Defects. <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	4
13311	Aromatic heterocyclic anion based ionic liquids and electrolytes. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 3502-3512.	1.3	7
13312	Benchmarking the computed proton solvation energy and absolute potential in non-aqueous solvents. <i>Electrochimica Acta</i> , 2023, 443, 141785.	2.6	2
13313	Multireference Wavefunction-Based Investigation of the Ground and Excited States of LrF and LrO. <i>Journal of Physical Chemistry A</i> , 2023, 127, 107-121.	1.1	2
13314	Anisotropically Fused Clusters Form a 2D Superatomic Sheet Exhibiting Polarized Light Emission. <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	3
13315	One-electron self-interaction error and its relationship to geometry and higher orbital occupation. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	5

#	ARTICLE	IF	CITATIONS
13352	Iridium-Catalyzed Chemo-, Diastereo-, and Enantioselective Allyl-Allyl Coupling: Accessing All Four Stereoisomers of (E)-Boryl-Substituted 1,5-Dienes by Chirality Pairing. <i>Angewandte Chemie</i> , 0, , .	1.6	0
13353	Molecular dynamics and Raman optical activity spectra reveal nucleotide conformation ratios in solution. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8198-8208.	1.3	6
13354	Comprehensive Computational Studies of Naturally Occurring Kuguacins as Antidiabetic Agents by Targeting Visfatin. <i>Chemistry Africa</i> , 2023, 6, 1415-1427.	1.2	8
13355	Magnetic anisotropy and structural flexibility in the field-induced single ion magnets [Co{(OPPh) ₂ (EPPH) ₂ N}] ₂ , E = S, Se, explored by experimental and computational methods. <i>Dalton Transactions</i> , 2023, 52, 2036-2050.	1.6	2
13356	Luminescence Spectral Properties of New Benzothiazole Polymethine Dye. <i>Journal of Applied Spectroscopy</i> , 2023, 89, 1021-1028.	0.3	2
13357	Machine learning based implicit solvent model for aqueous-solution alanine dipeptide molecular dynamics simulations. <i>RSC Advances</i> , 2023, 13, 4565-4577.	1.7	5
13358	Thymus satureoides Oil as Green Corrosion Inhibitor for 316L Stainless Steel in 3% NaCl: Experimental and Theoretical Studies. <i>Lubricants</i> , 2023, 11, 56.	1.2	6
13359	Valeramide and Halo-phenol in a Non-polar Liquid: DFT Based Characterization and Reactivity, Non-covalent Interaction, and Dielectric Relaxation Studies. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-26.	1.4	2
13360	A Molecular Dynamics and Quantum Mechanical Investigation of Intermolecular Interaction and Electron-transfer Mechanism between Copper-containing Nitrite Reductase and Redox Partner Pseudoazurin. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
13361	Thermodynamic and optical properties of HCOOH(H ₂ O) _n and HCOOH(NH ₃)(H ₂ O) _n clusters at various temperatures and pressures: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7869-7880.	1.3	1
13362	Thomas-Fermi and Other Density-Functional Theories. <i>Springer Handbooks</i> , 2023, , 297-308.	0.3	0
13363	Mechanism of Eu(III), La(III), Nd(III), and Th(IV) removal by g-C ₃ N ₄ based on spectroscopic analyses and DFT theoretical calculations. <i>Research on Chemical Intermediates</i> , 0, , .	1.3	1
13364	A Reactive Molecular Dynamics Study of Chlorinated Organic Compounds. Part I: Force Field Development. <i>ChemPhysChem</i> , 2023, 24, .	1.0	0
13365	Experimental and theoretical investigation of the effect of alkali (Li, Na and K) doping on the properties of nickel oxide thin films: Comparative study. <i>Main Group Chemistry</i> , 2024, 23, 73-88.	0.4	0
13366	Noncollinear density functional theory. <i>Physical Review Research</i> , 2023, 5, .	1.3	4
13368	Electronic structure and density functional theory. , 2023, , 3-35.		0
13369	A tetrathiafulvalene salt of the nitrite (NO ₂) ⁻ anion: investigations of the spin-Peierls phase. <i>Journal of Materials Chemistry C</i> , 0, , .	2.7	1
13370	Advances in the homogeneous catalyzed alcohols homologation: The mild side of the Guerbet reaction. A mini-review. <i>Catalysis Today</i> , 2023, 423, 114003.	2.2	5

#	ARTICLE	IF	CITATIONS
13371	Molecular Simulations on the Coalescence of Water-in-Oil Emulsion Droplets with Non-ionic Surfactant and Model Asphaltene. <i>Langmuir</i> , 2023, 39, 2233-2245.	1.6	2
13372	Interaction of a novel inorganic nickel complex with tyrosinase as potential inhibitor: Synthesis, spectroscopic, DFT, NBO, docking and ADMET properties. <i>Journal of Molecular Structure</i> , 2023, 1280, 134998.	1.8	0
13373	Electronic Effect on Phenoxide Migration at a Nickel(II) Center Supported by a Tridentate Bis(phosphinophenyl)phosphido Ligand. <i>Inorganic Chemistry</i> , 2023, 62, 3007-3017.	1.9	0
13374	DFT calculations reveal the origin of controllable synthesis of η^2 -boronyl carbonyl compounds from Cu/Pd-cocatalyzed four-component borocarbonylation of vinylarenes. <i>Catalysis Science and Technology</i> , 2023, 13, 2123-2133.	2.1	1
13375	A (TD-)DFT study on photo-NHC catalysis: photoenolization/Diels-Alder reaction of acid fluorides catalyzed by <i>N</i> -heterocyclic carbenes. <i>Chemical Science</i> , 2023, 14, 4027-4037.	3.7	2
13376	Designing molecules with a high-spin (quintet, $S = 2$) ground state for magnetic and spintronic applications. <i>Molecular Systems Design and Engineering</i> , 2023, 8, 874-886.	1.7	2
13377	A tris(2-aminoethyl)amine-based zinc complex as a highly water-soluble drug carrier for the anti-COVID-19 drug favipiravir: a joint experimental and theoretical study. <i>Dalton Transactions</i> , 2023, 52, 7031-7047.	1.6	3
13378	Combined experimental and DFT approach to BiNbO_4 polymorphs. <i>RSC Advances</i> , 2023, 13, 5576-5589.	1.7	5
13379	R2022: A DFT/MRCI Ansatz with Improved Performance for Double Excitations. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2011-2025.	1.1	5
13380	Molecular and electronic structure analysis of $[\text{Fe}(\text{CO})_4(\text{SiX})]$ ($X = \text{O}, \text{S}, \text{Se}$ and Te): a DFT study. <i>Journal of Chemical Sciences</i> , 2023, 135, .	0.7	4
13381	Synthesis and Optical Properties of a Series of Push-Pull Dyes Based on Pyrene as the Electron Donor. <i>Molecules</i> , 2023, 28, 1489.	1.7	1
13382	A Concerted Redox- and Light-Activated Agent for Controlled Multimodal Therapy against Hypoxic Cancer Cells. <i>Advanced Materials</i> , 2023, 35, .	11.1	8
13383	Kinetics, Products, and Mechanisms Study of the Atmospheric Degradation of (<i>E</i>)-4-Methoxy-3-buten-2-one with Hydroxyl Radicals. <i>ACS Earth and Space Chemistry</i> , 0, .	1.2	0
13384	Dihydropyrene/Cyclophanediene Photoswitching Mechanism Revisited with Spin-Flip Time-Dependent Density Functional Theory: Nature of the Photoisomerization Funnel at Stake!. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2921-2935.	1.1	3
13385	Modeling the Photo-Absorption Properties of Noble Metal Nanoclusters: A Challenge for Density-Functional Theory. <i>Journal of Physical Chemistry C</i> , 2023, 127, 7718-7729.	1.5	2
13386	Interaction of 5-Fluorouracil on the Surfaces of Pristine and Functionalized $\text{Ca}_{12}\text{O}_{12}$ Nanocages: An Intuition from DFT. <i>ACS Omega</i> , 2023, 8, 13551-13568.	1.6	9
13387	The Importance of Solvent Effects in Calculations of NMR Coupling Constants at the Doubles Corrected Higher Random-Phase Approximation. <i>Magnetochemistry</i> , 2023, 9, 102.	1.0	3
13388	LE and ICT properties of pyrazolo[1,5-a]pyrimidines based dyes: Experiments and DFT/TDDFT calculations. <i>Journal of Luminescence</i> , 2023, 257, 119772.	1.5	3

#	ARTICLE	IF	CITATIONS
13389	Physicochemical properties, drug likeness, ADMET, DFT studies, and in vitro antioxidant activity of oxindole derivatives. <i>Computational Biology and Chemistry</i> , 2023, 104, 107861.	1.1	7
13390	Towards understanding the interaction of quercetin with chitosan-phytate complex: An experimental and computational investigation. <i>Journal of Molecular Liquids</i> , 2023, 380, 121673.	2.3	0
13391	Understanding ion-ion and ion-urea interactions in mixtures of urea and choline oxyanions salts. <i>Journal of Molecular Liquids</i> , 2023, 379, 121647.	2.3	0
13392	Efficient tuning of various coumarin based donor dyes with diketopyrrolopyrrole by forming D-A π -A structure for high-efficiency solar cells: A DFT/ TD-DFT study. <i>Chemical Data Collections</i> , 2023, 45, 101017.	1.1	3
13393	Luminescent furo[2,3-c]isoquinolines as fluorophores - Tuning the luminophore by donor substitution. <i>Dyes and Pigments</i> , 2023, 214, 111190.	2.0	1
13394	Exploring the structural, photophysical and optoelectronic properties of a diaryl heptanoid curcumin derivative and identification as a SARS-CoV-2 inhibitor. <i>Journal of Molecular Structure</i> , 2023, 1281, 135110.	1.8	6
13395	Effect of strain on the effective mass of GaN and the mobility of AlGaN/GaN two-dimensional electron gas. <i>Materials Today Communications</i> , 2023, 35, 105788.	0.9	3
13396	Molecular structure of Ru(II)/diphosphine/4,6-dimethyl-2-pyrimidinethiol complexes: A combined experimental and density functional theory study. <i>Journal of Molecular Structure</i> , 2023, 1282, 135234.	1.8	0
13397	A molecular dynamics study on polybenzimidazole based proton exchange membrane with dual proton conductors. <i>Journal of Membrane Science</i> , 2023, 677, 121618.	4.1	4
13398	Atomic and close-to-atomic scale polishing of Lu ₂ O ₃ by plasma-assisted etching. <i>International Journal of Mechanical Sciences</i> , 2023, 252, 108374.	3.6	1
13399	Organytellurium(IV) complexes incorporating Schiff base ligand derived from 2-hydroxy-1-naphthaldehyde: Preparation, spectroscopic investigations, antimicrobial, antioxidant activities, DFT, MESP, NBO, molecular docking and ADMET evaluation. <i>Journal of Molecular Structure</i> , 2023, 1287, 135590.	1.8	11
13400	Single crystal structure of nitro terminated Azo Schiff base: DNA binding, antioxidant, enzyme inhibitory and photo-isomerization investigation. <i>Journal of Molecular Structure</i> , 2023, 1284, 135376.	1.8	1
13401	Thermal Half-Lives of Azobenzene Derivatives: Virtual Screening Based on Intersystem Crossing Using a Machine Learning Potential. <i>ACS Central Science</i> , 2023, 9, 166-176.	5.3	14
13402	Urethane formation in the presence of 2,2-dimorpholinodiethylether (DMDEE) and 1,4-dimethylpiperazine (DMP) – A combined experimental and theoretical study. <i>Computational and Theoretical Chemistry</i> , 2023, 1221, 114045.	1.1	5
13403	Electronic and optical properties of GaSe/ZnSe vdW heterojunction as photocatalyst by biaxial strain: A DFT study. <i>Chemical Physics Letters</i> , 2023, 814, 140333.	1.2	0
13404	Computational protocols for the 19F NMR parameters. Part 2: Fluorobenzenes. <i>Journal of Fluorine Chemistry</i> , 2023, 266, 110093.	0.9	1
13405	Efficient synthesis of chromeno[2,3-b]pyridine derivatives using Zn(OTf) ₂ as a catalyst: DFT computations, molecular docking and ADME studies. <i>Journal of Molecular Liquids</i> , 2023, 375, 121364.	2.3	5
13406	State Interaction Linear Response Time-Dependent Density Functional Theory with Perturbative Spin-Orbit Coupling: Benchmark and Perspectives. <i>Jacs Au</i> , 2023, 3, 358-367.	3.6	5

#	ARTICLE	IF	CITATIONS
13407	Sc-HOPO: A Potential Construct for Use in Radioscandium-Based Radiopharmaceuticals. <i>Inorganic Chemistry</i> , 2023, 62, 20567-20581.	1.9	5
13408	Benzodithiophene (BDT) and benzodiselenophene (BDSe) isomers' charge transport properties for organic optoelectronic devices. <i>Journal of Sulfur Chemistry</i> , 2023, 44, 462-478.	1.0	1
13409	Effects of dispersion corrections on the theoretical description of bulk metals. <i>Physical Review B</i> , 2023, 107, .	1.1	5
13410	HOAX: a hyperparameter optimisation algorithm explorer for neural networks. <i>Molecular Physics</i> , 0, , .	0.8	0
13411	Pyridinecarboxaldehydes: Structures, Vibrational Assignments and Molecular Characteristics Using Experimental and Theoretical Methods. <i>Brazilian Journal of Physics</i> , 2023, 53, .	0.7	3
13412	Thermal site energy fluctuations in photosystem I: new insights from MD/QM/MM calculations. <i>Chemical Science</i> , 2023, 14, 3117-3131.	3.7	1
13413	Molecular dynamics simulation studies of 1,3-dimethyl imidazolium nitrate ionic liquid with water. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	1
13414	Instigating the in vitro antidiabetic activity of new tridentate Schiff base ligand appended M(II) complexes: From synthesis, structural characterization, quantum computational calculations to molecular docking, and molecular dynamics simulation studies. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	23
13415	Copper(II) coordination polymer based on L-arginine as a supramolecular hybrid inorganic-organic material: synthesis, structural, spectroscopic and magnetic properties. <i>Research on Chemical Intermediates</i> , 2023, 49, 3563-3587.	1.3	3
13416	Structural Features Governing the Metabolic Stability of Tetraethyl-Substituted Nitroxides in Rat Liver Microsomes. <i>Antioxidants</i> , 2023, 12, 402.	2.2	5
13417	Computational and theoretical investigation of the geometrical structures, vibrational spectra and thermodynamic properties of the ionic and molecular clusters existing in vapours over strontium diiodide. <i>Molecular Physics</i> , 2023, 121, .	0.8	0
13418	On the self-consistency of DFT-1/2. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	0
13419	Mechanism of Calcium Permeation in a Glutamate Receptor Ion Channel. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 1293-1300.	2.5	8
13420	Benchmarking two-photon absorption strengths of rhodopsin chromophore models with CC3 and CCSD methodologies: An assessment of popular density functional approximations. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	2
13421	Toward Accurate Prediction of Ion Mobility in Organic Semiconductors by Atomistic Simulation. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1517-1528.	2.3	2
13422	Ultrafast optical limiting ability of <i>trans</i> -stilbene enhanced and broadened by a donor-acceptor structure. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7508-7518.	1.3	2
13423	A substrate descriptor based approach for the prediction and understanding of the regioselectivity in caged catalyzed hydroformylation. <i>Faraday Discussions</i> , 0, 244, 169-185.	1.6	2
13424	Mechanistic Insight into Cu-Catalyzed C-N Coupling of Hindered Aryl Iodides and Anilines Using a Pyrrol-ol Ligand Enables Development of Mild and Homogeneous Reaction Conditions. <i>ACS Catalysis</i> , 2023, 13, 2904-2915.	5.5	9

#	ARTICLE	IF	CITATIONS
13425	Benzothiazole and benzoxazole promoted cleavage of Ru(II)-C(aryl) bond in a four-membered ortho-metalated ruthenium(II) organometallics. <i>Structural Chemistry</i> , 2023, 28, 1709.	1.0	0
13426	Resonance Raman and Visible Micro-Spectroscopy for the In-Vivo and In-Vitro Characterization of Anthocyanin-Based Pigments in Blue and Violet Flowers: A Comparison with HPLC-ESI-MS Analysis of the Extracts. <i>Molecules</i> , 2023, 28, 1709.	1.7	0
13427	Diastereoselective Synthesis of Camptothecin-like Scaffolds: Construction of a New Class of Pseudo-natural Products. <i>European Journal of Organic Chemistry</i> , 2023, 26, .	1.2	0
13428	Mechanistic insights into the Cu(II)/DBU-catalyzed incorporation of CO ₂ into homopropargylic amines. <i>New Journal of Chemistry</i> , 2023, 47, 5691-5700.	1.4	0
13429	Theoretical investigation for dye-sensitized solar cells: effect of donor variation on the optoelectronic properties and charge transfer parameters. <i>Research on Chemical Intermediates</i> , 2023, 49, 1731-1754.	1.3	0
13430	Electrochemical Conversion of Cu Nanowire Arrays into Metal-Organic Frameworks HKUST-1. <i>Journal of the Electrochemical Society</i> , 2023, 170, 022506.	1.3	1
13431	Minimal Auxiliary Basis Set Approach for the Electronic Excitation Spectra of Organic Molecules. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 1968-1976.	2.1	5
13432	Cooperative CO ₂ adsorption mechanism in a perfluorinated Ce ^{IV} -based metal organic framework. <i>Journal of Materials Chemistry A</i> , 2023, 11, 5568-5583.	5.2	5
13433	Effect of crystal packing on charge transfer in the heteroleptic gallium(III) complex. <i>Russian Chemical Bulletin</i> , 2023, 72, 193-201.	0.4	8
13434	Cell Survival Enabled by Leakage of a Labile Metabolic Intermediate. <i>Molecular Biology and Evolution</i> , 2023, 40, .	3.5	2
13435	Binding profile of a mixed-ligand silver(I) complex with DNA and Topoisomerase I. <i>Computational Biology and Chemistry</i> , 2023, 103, 107831.	1.1	0
13436	The effect of long-range interactions on the infrared and Raman spectra of aragonite (CaCO ₃ , Pmcn) up to 25 GPa. <i>Scientific Reports</i> , 2023, 13, .	1.6	2
13437	A comprehensive DFT study on organosilicon-derived fungicide flusilazole and its germanium analogue: A computational approach to Si/Ge bioisosterism. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100939.	1.3	6
13438	Conformational analysis of amphetamine and methamphetamine: a comprehensive approach by vibrational and chiroptical spectroscopy. <i>Analyst</i> , 2023, 148, 1337-1348.	1.7	3
13439	The Impact of TPA Auxiliary Donor and the ĩ€-Linkers on the Performance of Newly Designed Dye-Sensitized Solar Cells: Computational Investigation. <i>Materials</i> , 2023, 16, 1611.	1.3	3
13440	Single Crystal Investigations, Hirshfeld Surface Analysis, DFT Studies, Molecular Docking, Physico-Chemical Characterization, and Biological Activity of a Novel Non-Centrosymmetric Compound with a Copper Transition Metal Precursor. <i>ACS Omega</i> , 2023, 8, 7738-7748.	1.6	3
13441	Synthesis and Biological Evaluation of Octahydroquinazolinones as Phospholipase A2, and Protease Inhibitors: Experimental and Theoretical Exploration. <i>Molecules</i> , 2023, 28, 1944.	1.7	1
13442	A Multifunctional Biomass Zinc Catalyst for Epoxy-Based Vitrimers and Composites. <i>European Polymer Journal</i> , 2023, 188, 111936.	2.6	1

#	ARTICLE	IF	CITATIONS
13443	Enabling Peculiar Photophysics and Mechanochromic Luminescence by Introducing Bromine in Push-Pull Pyridine Derivatives. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4176-4187.	1.5	1
13444	Synthesis, photophysical characterization, and aerobic redox reactivity of electron-rich tellurorhodamine photocatalysts. <i>Dalton Transactions</i> , 2023, 52, 3990-4001.	1.6	1
13445	Fluorinated Multi-Walled Carbon Nanotubes Coated Separator Mitigates Polysulfide Shuttle in Lithium-Sulfur Batteries. <i>Materials</i> , 2023, 16, 1804.	1.3	1
13446	Stable Room Temperature Nitrenes Created by Photolysis of Crystalline 4-Azido-2,3,5,6-tetrafluorobenzoic Acid. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4816-4824.	1.5	2
13447	Mechanism and Selectivity of Copper-Catalyzed Bromination of Distal C(sp ³)-H Bonds. <i>Organometallics</i> , 2023, 42, 2467-2476.	1.1	1
13448	Experimental and theoretical study of the low-temperature kinetics of the reaction of CN with CH ₂ O and implications for interstellar environments. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7719-7733.	1.3	4
13449	LC-MS Analysis, Computational Investigation, and Antimalarial Studies of <i>Andradite</i> Fruit. <i>Bioinformatics and Biology Insights</i> , 2023, 17, 117793222311549.	1.0	1
13450	Histidine oxidation in lytic polysaccharide monoxygenase. <i>Journal of Biological Inorganic Chemistry</i> , 2023, 28, 317-328.	1.1	8
13451	SEMICLASSICS: THE HIDDEN THEORY BEHIND THE SUCCESS OF DFT. <i>Lecture Notes Series, Institute for Mathematical Sciences</i> , 2023, , 179-249.	0.2	1
13452	Crystal Structure, Photophysical Study, Hirshfeld Surface Analysis, and Nonlinear Optical Properties of a New Hydroxyphenylamino Meldrum's Acid Derivative. <i>Molecules</i> , 2023, 28, 2181.	1.7	1
13453	DFT CALCULATIONS IN MONOMERIC AND DIMERIC FORMS OF N-BENZYLMALEIMIDE (NBM) COMBINED WITH VIBRATIONAL SPECTROSCOPIC PARAMETERS. <i>Eskişehir Teknik Üniversitesi Bilim Ve Teknoloji Dergisi B - Teorik Bilimler</i> , 0, , .	0.0	0
13454	Investigations on Novel 1,3-Diazetidene Based Four-Membered N-Heterocyclic Carbenes. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	0
13455	Hydrated electrons as nodes in porous clathrate hydrates. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	1
13456	Red-Fluorescing Paramagnetic Conjugated Polymer Nanoparticles of Triphenyl Methyl Radicals as Monomers in C-C Cross-Coupling Dispersion Polymerization. <i>Macromolecules</i> , 2023, 56, 2104-2112.	2.2	3
13457	Silicone nanomicelle dyeing method on polyester fibre: Comparative evaluation of chemical properties, fastness properties, and DFT. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100960.	1.3	3
13458	A deep investigation of NiO and MnO through the first principle calculations and Monte Carlo simulations. <i>Electronic Structure</i> , 0, , .	1.0	1
13459	An exotic 3-center/4-electron carbon-carbon pi long-bond: Is it tangible?. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	0
13460	Effect of intermolecular interaction of the charge-transfer complex between molecular tweezers and C ₆₀ /C ₇₀ on second-order nonlinear optical properties. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8799-8808.	1.3	0

#	ARTICLE	IF	CITATIONS
13461	Mechanism for the synthesis of medium-chain 1-alkenes from fatty acids catalyzed by binuclear iron UndA decarboxylase. <i>Journal of Catalysis</i> , 2023, 420, 123-133.	3.1	4
13462	Reactivity and Selectivity of the Diels-Alder Reaction of Anthracene in [Pd ₆ L ₄] ¹²⁺ Supramolecular Cages: A Computational Study. <i>Inorganic Chemistry</i> , 2023, 62, 4330-4340.	1.9	2
13463	Light-induced infrared difference spectroscopy on three different forms of orange carotenoid protein: focus on carotenoid vibrations. <i>Photochemical and Photobiological Sciences</i> , 0, , .	1.6	2
13464	Strongly constrained and appropriately normed density functional theory exchange-correlation functional applied to rare earth oxides. <i>Physical Review B</i> , 2023, 107, .	1.1	1
13465	Rupturing aromaticity by periphery overcrowding. <i>Nature Chemistry</i> , 2023, 15, 516-525.	6.6	11
13466	Unveiling the theoretical aspects of superelectrophilic activation in an inverse demand Diels-Alder reaction. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	0
13467	Oxidation Products from the Neolignan Licarin A by Biomimetic Reactions and Assessment of in vivo Acute Toxicity. <i>Planta Medica</i> , 0, , .	0.7	0
13468	A comparative study of the potential of [Os{(NHCH ₂ CH ₂) ₃ X}] catalysts (X = ¼N, P) for the reduction of dinitrogen to ammonia and hydrazine using FLP as a catalyst by density functional theory. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	0
13469	Synthesis, Structure, Hirshfeld Surface Analysis, Non-Covalent Interaction, and In Silico Studies of 4-Hydroxy-1-[(4-Nitrophenyl)Sulfonyl]Pyrrolidine-2-Carboxylic Acid. <i>Journal of Chemical Crystallography</i> , 2023, 53, 386-399.	0.5	2
13470	Fluids and Electrolytes under Confinement in Single-Digit Nanopores. <i>Chemical Reviews</i> , 2023, 123, 2737-2831.	23.0	32
13471	Double Hook Perylene Diimide as a New Receptor for PAHs: An Experimental and Theoretical Study. <i>ChemPhysChem</i> , 0, , .	1.0	0
13472	Synthesis of Sulfilimines Enabled by Copper-Catalyzed <i>S</i> -Arylation of Sulfenamides. <i>Journal of the American Chemical Society</i> , 2023, 145, 6310-6318.	6.6	26
13473	Robust Bio-derived Polyoxometalate Hybrid for Selective Aerobic Oxidation of Benzylic C(sp ³)-H Bonds. <i>ACS Catalysis</i> , 2023, 13, 4142-4154.	5.5	4
13474	DFT insights into competing mechanisms of guaiacol hydrodeoxygenation on a platinum cluster. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10460-10471.	1.3	3
13475	Classification of doubly excited molecular electronic states. <i>Chemical Science</i> , 2023, 14, 4012-4026.	3.7	5
13476	Dendrillic Acids A and B: Nitrogenous, Rearranged Spongian Nor-Diterpenes from a <i>Dendrilla</i> sp. Marine Sponge. <i>Journal of Natural Products</i> , 2023, 86, 482-489.	1.5	2
13477	Low-rank approximations for accelerating plane-wave hybrid functional calculations in unrestricted and noncollinear spin density functional theory. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	4
13478	Insights into selectivity of some oxygen containing gases by the CHCl ⁺ anion from molecular simulation. <i>Molecular Simulation</i> , 2023, 49, 758-768.	0.9	0

#	ARTICLE	IF	CITATIONS
13479	The study of the PES and the reaction mechanism between ketene and Lithium Carbenoids and the formation of cyclopropanone. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	0
13480	Investigation of the dual role of acyl phloroglucinols as a new hope for antibacterial and anti-SARS-CoV-2 agents employing integrated in vitro and multi-phase in silico approaches. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-18.	2.0	2
13481	Exciton States of Azobenzene Aggregates: A First Principles Study. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	2
13482	Reducing Exact Two-Component Theory for NMR Couplings to a One-Component Approach: Efficiency and Accuracy. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 2010-2028.	2.3	8
13483	Investigation of the N [^] C Ligand Effects on Emission Characteristics in a Series of Bis-Metalated [Ir(N [^] C)2(N [^] N)] ⁺ Complexes. <i>Molecules</i> , 2023, 28, 2740.	1.7	2
13484	Speciation of borate in aqueous solutions studied experimentally by potentiometry and Raman spectroscopy and computationally by DFT calculations. <i>New Journal of Chemistry</i> , 2023, 47, 8499-8506.	1.4	3
13485	Thiocarbohydrazone and Chalcone-Derived 3,4-Dihydropyrimidinethione as Lipid Peroxidation and Soybean Lipoxygenase Inhibitors. <i>ACS Omega</i> , 2023, 8, 11966-11977.	1.6	2
13487	Size-Reduced Basis Set Calculation of Accurate Isotropic Nuclear Magnetic Shieldings Using CTOCD-GRRO and GPRO Methods in Amino Acids and Oligopeptides. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3036-3047.	1.1	0
13488	Electrostatic Potential for Exploring Electron Delocalization in Infinitenes, Circulenes, and Nanobelts. <i>Journal of Organic Chemistry</i> , 2023, 88, 4123-4133.	1.7	3
13489	The essential role of symmetry in understanding ³ He chemical shifts in endohedral helium fullerenes. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10620-10627.	1.3	3
13490	Computational Modelling of MOF Mechanics: From Elastic Behaviour to Phase Transformations. , 2023, , 113-204.		0
13491	SPECTRAL-LUMINESCENT PROPERTIES OF A NEW BENZETHIAZOLE POLYMETHINE DYE. , 2022, 89, 762-769.		0
13492	Thermal isomerization of phenylazoindoles: Inversion or rotation? That is the question. <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	2
13493	Design, Synthesis, Computational Investigations, and Antitumor Evaluation of <i>N</i> -Rhodanine Glycosides Derivatives as Potent DNA Intercalation and Topo II Inhibition against Cancer Cells. <i>ACS Omega</i> , 2023, 8, 13300-13314.	1.6	1
13494	On the computation of frequency dependent molecular magnetizabilities via dynamical charge and current electron densities. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	1
13495	Complexes of a model trimeric acylphloroglucinol with a Cu ²⁺ ion: a DFT study. <i>ChemistrySelect</i> , 2023, .	0.7	0
13496	Charge Localization in Acene Crystals from <i>Ab Initio</i> Electronic Structure. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 3343-3351.	2.1	2
13497	Synthesis of Novel 2,9-Disubstituted-6-morpholino Purine Derivatives Assisted by Virtual Screening and Modelling of Class I PI3K Isoforms. <i>Polymers</i> , 2023, 15, 1703.	2.0	1

#	ARTICLE	IF	CITATIONS
13498	Copper(II)â€TEMPO Interaction. Israel Journal of Chemistry, 0, , .	1.0	0
13499	How Metal Nuclearity Impacts Electrocatalytic H ₂ Production in Thiocarbohydrazone-Based Complexes. Inorganics, 2023, 11, 149.	1.2	0
13500	Predicting power conversion efficiency of binary organic solar cells based on Y6 acceptor by machine learning. Journal of Energy Chemistry, 2023, 82, 139-147.	7.1	7
13501	Ring-opening reactions of phosphoramidate heterocycles. Tetrahedron, 2023, 137, 133390.	1.0	1
13502	Energy level alignments between organic and inorganic layers in 2D layered perovskites: conjugation <i>vs</i>. substituent. Nanoscale, 0, , .	2.8	0
13503	Importance of spin-triplet excited-state character in the reverse intersystem crossing process of spiro-based TADF emitters. Journal of Materials Chemistry C, 2023, 11, 6119-6129.	2.7	1
13504	Coordination vs. Insertion: On the Interaction of 5dâ€Transition Metal Carbonyl Clusters with Silver(I). Chemistry - A European Journal, 0, , .	1.7	2
13505	Cost-Effective Simulations of Vibrationally-Resolved Absorption Spectra of Fluorophores with Machine-Learning-Based Inhomogeneous Broadening. Journal of Chemical Theory and Computation, 2023, 19, 2304-2315.	2.3	5
13506	Computational evaluation on molecular stability and binding affinity of methyl dopa against Lysine-specific demethylase 4D Enzyme through quantum chemical computations and molecular docking analysis. Journal of Molecular Structure, 2023, 1286, 135518.	1.8	6
13507	Accurate Interaction Energies of CO₂ with the 20 Naturally Occurring Amino Acids. ChemPhysChem, 2023, 24, .	1.0	0
13508	Elucidating the Role of Noncovalent Interactions in Favipiravir, a Drug Active against Various Human RNA Viruses; a 1H-14N NQDR/Periodic DFT/QTAIM/RDS/3D Hirshfeld Surfaces Combined Study. Molecules, 2023, 28, 3308.	1.7	4
13509	Meta-GGA SCAN Functional in the Prediction of Ground State Properties of Magnetic Materials: Review of the Current State. Metals, 2023, 13, 728.	1.0	5
13510	MOF-derived Co/Fe@NPC-500 with large amounts of low-valent metals as an electro-Fenton cathode for efficient degradation of ceftazidime. Applied Catalysis B: Environmental, 2023, 333, 122755.	10.8	21
13511	Synthesis, Computational Studies, Molecular Docking, Antiâ€inflammatory and Antioxidant Activities of Î±â€Aminophosphonates Incorporating an Azo Chromophore for Polyester Printing Application. ChemistrySelect, 2023, 8, .	0.7	1
13512	Reactivity Factors in Catalytic Methanogenesis and Their Tuning upon Coenzyme F430 Biosynthesis. Journal of the American Chemical Society, 2023, 145, 9039-9051.	6.6	1
13513	Unraveling the dependence of proton transfer on solvent polarity in ion pairs of carbamates and dithiocarbamates with nitrogenâ€based counterions. Journal of Physical Organic Chemistry, 2023, 36, .	0.9	1
13514	Conjugation of a Silver-Based Coordination Polymer with Curcumin: A New Case of an Inorganic Polymeric Co-crystal. Crystal Growth and Design, 0, , .	1.4	0
13515	High Valent Mercury Fluoride Ions. ChemPhysChem, 0, , .	1.0	0

#	ARTICLE	IF	CITATIONS
13517	Investigation of Solvent Effect and H-Bonding on Spectroscopic Properties of 1-(3-Amino-6-(2,5-dichlorothiophen-3-yl)-4-phenylfuro[2,3-b]Pyridin-2-yl) Ethenone: Experimental and Computational Study. <i>Journal of Fluorescence</i> , 2023, 33, 2349-2360.	1.3	0
13518	Virtual screening of organic quinones as cathode materials for sodium-ion batteries. <i>Energy Advances</i> , 2023, 2, 820-828.	1.4	3
13519	Newly designed triazatruxene-based dye-sensitized solar cells containing different benzothiazine I€-linkers: Geometric, optoelectronic, charge transfer properties, and cyanoacrylic acid versus benzoic acid. <i>Computational and Theoretical Chemistry</i> , 2023, 1224, 114127.	1.1	2
13520	On the antiaromatic-aromatic-antiaromatic transition of the stacked cyclobutadiene dimer. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
13521	Formation and Reactivity of NHC-Boryl Radicals: Insight into Substituent Effect from Theoretical Calculations. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
13522	Control and regulation of the performance of fullerene-based dye-sensitized solar cells with D-D-A structure by external electric fields. <i>Nanoscale Advances</i> , 0, , .	2.2	1
13523	Constrained density functional theory calculations for estimation of forward and backward intermolecular charge transfer energy. <i>Bulletin of the Korean Chemical Society</i> , 0, , .	1.0	0
13524	Synthesis, spectroscopic, crystallographic, quantum and molecular docking investigations of cis-4,5-diphenylimidazolidine-2-thione. <i>Journal of Molecular Structure</i> , 2023, 1286, 135633.	1.8	16
13525	An experimental and theoretical investigation of the N(² D) + C ₆ H ₆ (benzene) reaction with implications for the photochemical models of Titan. <i>Faraday Discussions</i> , 0, 245, 327-351.	1.6	4
13526	A Combined Experimental and Computational (DFT, RDF, MC and MD) Investigation of Epoxy Resin as a Potential Corrosion Inhibitor for Mild Steel in a 0.5 M H ₂ SO ₄ Environment. <i>Polymers</i> , 2023, 15, 1967.	2.0	8
13557	Computational Approaches for Organic Semiconductors: From Chemical and Physical Understanding to Predicting New Materials. <i>Chemical Reviews</i> , 2023, 123, 7498-7547.	23.0	11
13562	The Fully Oxidized State of the Glutamate Coordinated O ₂ -Tolerant [NiFe]-Hydrogenase Shows a Ni(III)/Fe(III) Open-Shell Singlet Ground State. <i>Journal of the American Chemical Society</i> , 2023, 145, 10954-10959.	6.6	3
13576	Electron-density-based analysis and electron density functional theory (DFT) methods. , 2023, , 177-197.		0
13577	Electron density to analyze acids and bases of Lewis: computational tools. , 2023, , 313-333.		0
13579	Conceptual Ruedenberg theory of chemical bonds: the necessary step beyond conceptual DFT. , 2023, , 113-175.		0
13582	Predicting reactivity with a general-purpose reactivity indicator. , 2023, , 159-180.		1
13605	Benchmarking Modern Density Functionals for Broad Applications in Chemistry. , 2024, , 78-93.		0
13643	Density-functional theory for electronic excited states. , 2023, , 69-118.		7

#	ARTICLE	IF	CITATIONS
13644	Fluorescent proteins. , 2023, , 337-349.		1
13686	Application of Molecular Simulation Methods in Treating Intrinsic Structures of Energetic Materials. , 2023, , 41-113.		1
13690	Computational Investigation of $\text{Ti}(\text{H}_2\text{O})_2 + \text{C}_2\text{H}_4$ and $\text{Ti}(\text{H}_2\text{O})_2 + \text{CH}_2\text{CHCN}$ Reactions: Benchmark Analysis and Implications for Titan's Atmosphere. Lecture Notes in Computer Science, 2023, , 705-717.	1.0	0
13710	Electronic structure in organic dye-sensitized solar cells: Insight from density functional theory and electron dynamics. Advances in Quantum Chemistry, 2023, , .	0.4	0
13712	Computing and Compressing Electron Repulsion Integrals on FPGAs. , 2023, , .		1
13731	Review of Approximations for the Exchange-Correlation Energy in Density-Functional Theory. , 2023, , 1-90.		3
13756	Atomistic simulation analysis of plasma surface activation in wafer-to-wafer oxide fusion bonding. , 2023, , .		0
13788	Electronic current densities and origin-independent property densities induced by optical fields. Physical Chemistry Chemical Physics, 0, , .	1.3	0
13838	Computational Insights of Dimensional Organic Materials. , 2023, , 382-473.		2
13880	Relativistic Real-Time Methods. , 2024, , 200-228.		0
13886	Gas Phase IR Spectra of Hydrogen Functionalised Pentacene. Thirty Years of Astronomical Discovery With UKIRT, 2023, , 209-214.	0.3	0
13887	Some phosphonic compounds as DSSCs via DFT/TDDFT theoretical quantum investigations. AIP Conference Proceedings, 2023, , .	0.3	0
13894	Machine-Learning for Static and Dynamic Electronic Structure Theory. Challenges and Advances in Computational Chemistry and Physics, 2023, , 113-160.	0.6	0
13942	Non-empirical quadratic-integrand double-hybrid (QIDH) functionals. Annual Reports in Computational Chemistry, 2023, , 87-119.	0.9	0
13991	Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry with Re-Engineered 2, a 5-Dihydroxypheny Acid Derivative. , 2024, , 313-337.		0
14003	Distinct Roles of the Principal Exchange-Correlation Energy and the Secondary Correlation Energy Functionals in the MGC-SDFT-UHFD Decoupling. , 0, , .		0
14017	Prediction of Structural and Electronic Properties of Doped Compounds $\text{Ca}_{0.75}\text{X}_{0.25}\text{B}_2$ ($\text{X} = \text{Fe}, \text{Cd}, \text{K}$) Using Density Functional Theory. Journal of Electronic Materials, 0, , .	1.0	0
14023	Quantum-Chemical Methods. Lecture Notes in Quantum Chemistry II, 2023, , 7-33.	0.3	0

#	ARTICLE	IF	CITATIONS
14048	Theoretical and Experimental Study of the Chemical Modification of Poly(epichlorohydrin) by Grafting Menthol. , 0, , .		0
14074	Effect of Different Basis Sets on the Theoretical Calculation of Zinc Isotope Fractionation of Zn Complexes. <i>Advances in Science, Technology and Innovation</i> , 2023, , 113-115.	0.2	0
14102	The Structures and the Vibrational Frequencies of Organic Cd Complexes with Forced Symmetry. <i>Advances in Science, Technology and Innovation</i> , 2023, , 175-177.	0.2	0
14113	Synthesis of SiN/SiS-heterocycles <i>via</i> the reactions of a bis-silylene with isocyanate/isothiocyanate molecules. <i>Chemical Communications</i> , 2024, 60, 1148-1151.	2.2	0