Development of density functionals for thermochemica

Journal of Chemical Physics

121, 3405-3416

DOI: 10.1063/1.1774975

Citation Report

#	Article	IF	Citations
17	Theoretische Chemie 2004. Nachrichten Aus Der Chemie, 2005, 53, 287-293.	0.0	1
18	Is there a satisfactory description of the molecular structure of Roeskyâ€™s ketone?. Chemical Physics Letters, 2005, 413, 440-444.	1.2	11
19	Benchmark Databases for Nonbonded Interactions and Their Use To Test Density Functional Theory. Journal of Chemical Theory and Computation, 2005, 1, 415-432.	2.3	832
20	Carbon Nanotube Inner Phase Chemistry:Â The Cl-Exchange SN2 Reaction. Nano Letters, 2005, 5, 1861-1866.	4.5	31
21	Benchmarking approximate density functional theory. I.s/d excitation energies in 3d transition metal cations. Journal of Computational Chemistry, 2005, 26, 1505-1518.	1.5	57
22	Assessment of various density functionals and basis sets for the calculation of molecular anharmonic force fields. International Journal of Quantum Chemistry, 2005, 104, 830-845.	1.0	67
23	Comparative studies of the spectroscopy of CuCl2: DFT versus standard ab initio approaches. Journal of Chemical Physics, 2005, 122, 164306.	1.2	24
24	The infrared spectrum of Auâˆ’âˆ™CO2. Journal of Chemical Physics, 2005, 122, 154301.	1.2	56
25	Correlation energy functionals dependent on an effective number of electrons: Charged species and equilibrium geometries. Journal of Chemical Physics, 2005, 123, 144111.	1.2	0
26	A phase-space approach to the T1â‡0 radiationless decay in benzene: The effect of deuteration. Journal of Chemical Physics, 2005, 123, 074304.	1.2	10
27	Progress in the development of exchange-correlation functionals. , 2005, , 669-724.		108
28	Chapter 3 Computational Thermochemistry: A Brief Overview of Quantum Mechanical Approaches. Annual Reports in Computational Chemistry, 2005, 1, 31-43.	0.9	46
29	Hole localization in [AlO4]0 defects in silica materials. Journal of Chemical Physics, 2005, 122, 144704.	1.2	74
30	Photoelectron Spectra and Ion Chemistry of Imidazolideâ€. Journal of Physical Chemistry A, 2005, 109, 11504-11514.	1.1	52
31	Benchmark Calculations of Reaction Energies, Barrier Heights, and Transition-State Geometries for Hydrogen Abstraction from Methanol by a Hydrogen Atom. Journal of Physical Chemistry A, 2005, 109, 773-778.	1.1	57
32	Anharmonic force fields and thermodynamic functions using density functional theory. Molecular Physics, 2005, 103, 863-876.	0.8	59
33	Design of Density Functionals That Are Broadly Accurate for Thermochemistry, Thermochemical Kinetics, and Nonbonded Interactions. Journal of Physical Chemistry A, 2005, 109, 5656-5667.	1.1	1,451
34	Trends in Râˆ’X Bond Dissociation Energies (R = Me, Et,i-Pr,t-Bu; X = H, CH3, OCH3, OH, F):Â A Surprising Shortcoming of Density Functional Theory. Journal of Physical Chemistry A, 2005, 109, 7558-7566.	1.1	210

#	Article	IF	Citations
35	Assessment of Recently Developed Multicoefficient Strategies for the Treatment of Ï€-Conjugated Molecules. Journal of Physical Chemistry A, 2005, 109, 3470-3475.	1.1	26
36	Platinum Stilbazoles:Â Ring-Walking Coupled with Arylâ^'Halide Bond Activation. Journal of the American Chemical Society, 2005, 127, 9322-9323.	6.6	60
37	Bond Dissociation Energies and Radical Stabilization Energies Associated with Model Peptide-Backbone Radicals. Journal of Physical Chemistry A, 2005, 109, 6318-6325.	1.1	72
38	Modeling Î²-Scission Reactions of Peptide Backbone Alkoxy Radicals:Â Backbone Câ^'C Bond Fission. Journal of Chemical Theory and Computation, 2005, 1, 889-899.	2.3	6
39	Benchmark Database of Barrier Heights for Heavy Atom Transfer, Nucleophilic Substitution, Association, and Unimolecular Reactions and Its Use to Test Theoretical Methods. Journal of Physical Chemistry A, 2005, 109, 2012-2018.	1.1	736
40	Activation Energies of Pericyclic Reactions:Â Performance of DFT, MP2, and CBS-QB3 Methods for the Prediction of Activation Barriers and Reaction Energetics of 1,3-Dipolar Cycloadditions, and Revised Activation Enthalpies for a Standard Set of Hydrocarbon Pericyclic Reactions. Journal of Physical Chemistry A, 2005, 109, 9542-9553.	1.1	233
41	Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions. Journal of Chemical Physics, 2005, 123, 161103.	1.2	979
42	Semiempirical hybrid functional with improved performance in an extensive chemical assessment. Journal of Chemical Physics, 2005, 123, 121103.	1.2	131
43	Importance of short-range versus long-range Hartree-Fock exchange for the performance of hybrid density functionals. Journal of Chemical Physics, 2006, 125, 074106.	1.2	823
44	Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2006, 110, 13624-13631.	1.1	41
45	Comparative assessment of density functional methods for 3d transition-metal chemistry. Journal of Chemical Physics, 2006, 124, 224105.	1.2	180
46	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. Journal of Chemical Physics, 2006, 124, 094108.	1.2	122
47	Assessing a new nonempirical density functional: Difficulties in treating Ï€-conjugation effects. Journal of Chemical Physics, 2006, 124, 124112.	1.2	34
48	Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2006, 2, 364-382.	2.3	3,329
49	Comparative DFT Study of van der Waals Complexes:Â Rare-Gas Dimers, Alkaline-Earth Dimers, Zinc Dimer, and Zinc-Rare-Gas Dimers. Journal of Physical Chemistry A, 2006, 110, 5121-5129.	1.1	706
50	Assessment of a long-range corrected hybrid functional. Journal of Chemical Physics, 2006, 125, 234109.	1.2	1,526
51	On the accuracy of density functional theory in transition metal chemistry. Annual Reports on the Progress of Chemistry Section C, 2006, 102, 203.	4.4	285
52	Benchmark Study of DFT Functionals for Late-Transition-Metal Reactionsâ€. Journal of Physical Chemistry A, 2006, 110, 709-716.	1.1	223

#	Article	IF	Citations
53	Geometries of Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2006, 2, 1282-1290.	2.3	557
54	Transfer hydrogenation between ethane and ethene: a critical assessment of theoretical procedures. Molecular Physics, 2006, 104, 777-794.	0.8	12
55	Assessment of Several Hybrid DFT Functionals for the Evaluation of Bond Length Alternation of Increasingly Long Oligomers. Journal of Physical Chemistry A, 2006, 110, 5952-5959.	1.1	77
56	A Single Transition State Serves Two Mechanisms. The Branching Ratio for CH2Oâ€¢-+ CH3Cl on Improved Potential Energy Surfaces. Journal of Physical Chemistry A, 2006, 110, 2801-2806.	1.1	20
57	Assessment of Density Functionals for Ï€ Systems:Â Energy Differences between Cumulenes and Poly-ynes; Proton Affinities, Bond Length Alternation, and Torsional Potentials of Conjugated Polyenes; and Proton Affinities of Conjugated Shiff Bases. Journal of Physical Chemistry A, 2006, 110, 10478-10486.	1.1	196
58	Thermochemistry of Acetonyl and Related Radicals. Journal of Physical Chemistry A, 2006, 110, 13618-13623.	1.1	52
59	Effect of Side Chains on Competing Pathways for Î²-Scission Reactions of Peptide-Backbone Alkoxyl Radicals. Journal of Physical Chemistry A, 2006, 110, 10316-10323.	1.1	19
60	Rozen's Epoxidation Reagent, CH3CNÂ·HOF:Â A Theoretical Study of Its Structure, Vibrational Spectroscopy, and Reaction Mechanismâ€. Journal of Physical Chemistry A, 2006, 110, 8275-8281.	1.1	9
61	Reliable Low-Cost Theoretical Procedures for Studying Additionâ^'Fragmentation in RAFT Polymerization. Journal of Physical Chemistry A, 2006, 110, 2486-2492.	1.1	85
62	PdnCO (n= 1,2):Â Accurate Ab Initio Bond Energies, Geometries, and Dipole Moments and the Applicability of Density Functional Theory for Fuel Cell Modeling. Journal of Physical Chemistry B, 2006, 110, 24030-24046.	1.2	45
63	Density Functional for Spectroscopy:Â No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States. Journal of Physical Chemistry A, 2006, 110, 13126-13130.	1.1	1,140
64	A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. Journal of Chemical Physics, 2006, 125, 194101.	1.2	4,175
65	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
66	An Assessment of Theoretical Procedures for Predicting the Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Benzene. Journal of Physical Chemistry A, 2006, 110, 8942-8951.	1.1	70
67	Modeling the Kinetics of Bimolecular Reactions. Chemical Reviews, 2006, 106, 4518-4584.	23.0	533
68	Semiempirical hybrid density functional with perturbative second-order correlation. Journal of Chemical Physics, 2006, 124, 034108.	1.2	2,729
69	Characterization of synthetic oxomanganese complexes and the inorganic core of the O2-evolving complex in photosystem II: Evaluation of the DFT/B3LYP level of theory. Journal of Inorganic Biochemistry, 2006, 100, 786-800.	1.5	99
70	Semiempirical GGA-type density functional constructed with a long-range dispersion correction. Journal of Computational Chemistry, 2006, 27, 1787-1799.	1.5	24,222

#	Article	IF	Citations
71	Hydrocarbon Bond Dissociation Enthalpies: From Substituted Aromatics to Large Polyaromatics. ChemPhysChem, 2006, 7, 2205-2214.	1.0	45
72	Growing Graphene Sheets from Reactions with Methyl Radicals: A Quantum Chemical Study. ChemPhysChem, 2006, 7, 1770-1778.	1.0	22
73	Rearrangements in Model Peptide-Type Radicalsvia Intramolecular Hydrogen-Atom Transfer. Helvetica Chimica Acta, 2006, 89, 2254-2272.	1.0	39
74	Combined valence bond-molecular mechanics potential-energy surface and direct dynamics study of rate constants and kinetic isotope effects for the H+C2H6 reaction. Journal of Chemical Physics, 2006, 124, 044315.	1.2	47
75	The electronic spectrum of AgCl2: Ab initio benchmark versus density-functional theory calculations on the lowest ligand-field states including spin-orbit effects. Journal of Chemical Physics, 2006, 124, 034307.	1.2	11
76	Polymerization, shock cooling, and the high-pressure phase diagram of nitrogen. Physical Review B, 2006, 74, .	1.1	40
77	A thermochemically competitive local hybrid functional without gradient corrections. Journal of Chemical Physics, 2007, 126, 011103.	1.2	113
78	Photodissociation dynamics of the 2-propyl radical, C3H7. Journal of Chemical Physics, 2007, 126, 144302.	1.2	27
79	Towards a Better Understanding of 'Delocalized Charge' in Ionic Liquid Anions. Australian Journal of Chemistry, 2007, 60, 15.	0.5	79
80	AB INITIO MOLECULAR DYNAMICS STUDY OF DISSOLVED SiO2 IN SUPERCRITICAL WATER. Journal of Theoretical and Computational Chemistry, 2007, 06, 49-62.	1.8	18
81	Local hybrid functionals based on density matrix products. Journal of Chemical Physics, 2007, 127, 164117.	1.2	54
82	General Performance of Density Functionals. Journal of Physical Chemistry A, 2007, 111, 10439-10452.	1.1	907
83	Assessment of long-range corrected functionals performance for nâ†'Ï€* transitions in organic dyes. Journal of Chemical Physics, 2007, 127, 094102.	1.2	119
84	Carbonâˆ'Hydrogen Bond Activation in Hydridotris(pyrazolyl)borate Platinum(IV) Complexes:â€‰ Comparison of Density Functionals, Basis Sets, and Bonding Patterns. Journal of Chemical Theory and Computation, 2007, 3, 2268-2281.	2.3	14
85	How Well Can New-Generation Density Functionals Describe Protonated Epoxides Where Older Functionals Fail?. Journal of Organic Chemistry, 2007, 72, 295-298.	1.7	41
86	Density Functional Theory Study of Free-Radical Polymerization of Acrylates and Methacrylates:Â Structureâˆ'Reactivity Relationship. Macromolecules, 2007, 40, 9590-9602.	2.2	40
87	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. Journal of Chemical Physics, 2007, 126, 144105.	1.2	290
88	Bond Dissociation Energies and Radical Stabilization Energies:â€‰ An Assessment of Contemporary Theoretical Procedures. Journal of Physical Chemistry A, 2007, 111, 13638-13644.	1.1	101

#	Article	IF	Citations
89	Multicoefficient Gaussian-3 Calculation of the Rate Constant for the OH + CH4Reaction and Its12C/13C Kinetic Isotope Effect with Emphasis on the Effects of Coordinate System and Torsional Treatment. Journal of Physical Chemistry A, 2007, 111, 11706-11717.	1.1	30
90	Modeling elementary reactions in coke formation from first principles. Molecular Simulation, 2007, 33, 879-887.	0.9	32
91	Analytic derivatives for perturbatively corrected â€œdouble hybridâ€•density functionals: Theory, implementation, and applications. Journal of Chemical Physics, 2007, 126, 124115.	1.2	173
92	Theoretical Study of the Thermodynamics and Kinetics of Hydrogen Abstractions from Hydrocarbons. Journal of Physical Chemistry A, 2007, 111, 11771-11786.	1.1	134
93	Theoretical Study of Solvent Effects on the Thermodynamics of Iron(III) [Tetrakis(pentafluorophenyl)]porphyrin Chloride Dissociation. Journal of Physical Chemistry B, 2007, 111, 10992-10998.	1.2	10
94	Benchmark Calculations on the Electron Detachment Energies of MO₃⁻ and M₂O₆⁻ (M = Cr, Mo, W). Journal of Physical Chemistry A, 2007, 111, 11908-11921.	1.1	67
95	Improved meta-GGA Correlation Functional of the Lap Family. Journal of Chemical Theory and Computation, 2007, 3, 746-754.	2.3	9
96	Ab Initio Study of Free-Radical Polymerization:Â Defect Structures in Poly(vinyl chloride). Macromolecules, 2007, 40, 1321-1331.	2.2	47
97	Density Functional Theory Investigation of Competitive Free-Radical Processes during the Thermal Cracking of Methylated Polyaromatics: Estimation of Kinetic Parameters. Journal of Physical Chemistry A, 2007, 111, 3082-3090.	1.1	21
98	Ab Initio Thermochemistry and Kinetics for Carbon-Centered Radical Addition and Î²-Scission Reactions. Journal of Physical Chemistry A, 2007, 111, 8416-8428.	1.1	67
99	Ab Initio, Density Functional Theory, and Continuum Solvation Model Prediction of the Product Ratio in the SN2 Reaction of NO2-with CH3CH2Cl and CH3CH2Br in DMSO Solution. Journal of Physical Chemistry A, 2007, 111, 10068-10074.	1.1	21
100	Representative Benchmark Suites for Barrier Heights of Diverse Reaction Types and Assessment of Electronic Structure Methods for Thermochemical Kinetics. Journal of Chemical Theory and Computation, 2007, 3, 569-582.	2.3	207
101	Global DFT-Based Reactivity Indicators:â€‰ An Assessment of Theoretical Procedures in Zeolite Catalysis. Journal of Physical Chemistry C, 2007, 111, 3028-3037.	1.5	14
102	Oâ˜H Bond Dissociation Enthalpies of Oximes:â€‰ A Theoretical Assessment and Experimental Implications. Journal of Physical Chemistry A, 2007, 111, 13112-13125.	1.1	34
103	Thermochemical Kinetics of Hydrogen-Atom Transfers between Methyl, Methane, Ethynyl, Ethyne, and Hydrogen. Journal of Physical Chemistry A, 2007, 111, 4632-4642.	1.1	59
104	Should Contemporary Density Functional Theory Methods Be Used to Study the Thermodynamics of Radical Reactions?. Journal of Physical Chemistry A, 2007, 111, 10754-10768.	1.1	140
105	Comparison of Density Functionals for Reactions of Sulfur Ylides with Aldehydes and Olefins. Journal of Physical Chemistry A, 2007, 111, 12019-12025.	1.1	9
106	Low-Lying Electronic States of M₃O₉⁻ and M₃O₉²⁻ (M = Mo, W). Journal of Physical Chemistry A, 2007, 111, 11093-11099.	1.1	47

#	Article	IF	Citations
107	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. Physical Review B, 2007, 75, .	1.1	306
108	How to Compute Isomerization Energies of Organic Molecules with Quantum Chemical Methods. Journal of Organic Chemistry, 2007, 72, 2118-2126.	1.7	234
109	Local hybrid functionals: An assessment for thermochemical kinetics. Journal of Chemical Physics, 2007, 127, 194102.	1.2	87
110	Basis Set Limit Coupled Cluster Study of H-Bonded Systems and Assessment of More Approximate Methods. Journal of Physical Chemistry A, 2007, 111, 11122-11133.	1.1	87
111	An Evaluation of Harmonic Vibrational Frequency Scale Factors. Journal of Physical Chemistry A, 2007, 111, 11683-11700.	1.1	2,264
112	Theoretical Study of the Oxidation CatalystN-Hydroxyphthalimide (NHPI):â€‰ Thermochemical Properties, Internal Rotor Potential, and Gas- and Liquid-Phase Bond Dissociation Energies. Journal of Physical Chemistry C, 2007, 111, 5760-5765.	1.5	36
113	Density Functionals for Noncovalent Interaction Energies of Biological Importance. Journal of Chemical Theory and Computation, 2007, 3, 289-300.	2.3	557
114	Geometries of Second-Row Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 2234-2242.	2.3	154
115	Density Functional Theory Study of the Formation of Naphthalene and Phenanthrene from Reactions of Phenyl with Vinyl- and Phenylacetylene. Journal of Chemical Theory and Computation, 2007, 3, 139-145.	2.3	28
116	Proton Walk in the Aqueous Platinum Complex [TpPtMeCO] via a Sticky Ïƒ-Methane Ligand. Chemistry - A European Journal, 2007, 13, 2812-2823.	1.7	13
117	DFT and ab initio calculations on two reactions between hydrogen atoms and the fire suppressants 2-H heptafluoropropane and CF3 Br. Journal of Computational Chemistry, 2007, 28, 1582-1592.	1.5	14
118	Fluorinated Furanâ€2(5H)â€ones: Reactivity and Stereoselectivity in Dielsâ€“Alder Reactions. European Journal of Organic Chemistry, 2007, 2007, 5101-5111.	1.2	15
119	Ab Initio Study of Poly(vinyl chloride) Propagation Kinetics: Head-to-Head versus Head-to-Tail Additions. ChemPhysChem, 2007, 8, 541-552.	1.0	26
120	Local hybrid exchange-correlation functionals based on the dimensionless density gradient. Chemical Physics Letters, 2007, 440, 160-168.	1.2	98
121	How useful are reactivity indicators for the description of hydrogen abstraction reactions on polycyclic aromatic hydrocarbons?. Chemical Physics Letters, 2007, 444, 17-22.	1.2	12
122	Initiation of petroleum formation and antioxidant function â€“ a DFT study of sulfurï£¿sulfur bond dissociation enthalpies. Journal of Physical Organic Chemistry, 2007, 20, 754-763.	0.9	4
123	Thermochemistry, Bond Energies, and Internal Rotor Potentials of Dimethyl Tetraoxide. Journal of Physical Chemistry A, 2007, 111, 12026-12036.	1.1	14
124	Long-range corrected density functional study on weakly bound systems: Balanced descriptions of various types of molecular interactions. Journal of Chemical Physics, 2007, 126, 234114.	1.2	135

#	Article	IF	Citations
125	Reparameterization of a meta-generalized gradient approximation functional by combining TPSS exchange with Ï„1 correlation. Theoretical Chemistry Accounts, 2007, 118, 693-707.	0.5	19
126	Hybrid exchange correlation functionals and potentials: Concept elaboration. Journal of Structural Chemistry, 2007, 48, S1-S31.	0.3	40
127	Assessment of density-functional models for organic molecular semiconductors: The role of Hartreeâ€“Fock exchange in charge-transfer processes. Chemical Physics, 2007, 331, 321-331.	0.9	63
128	Two theoretical simulations of hydrocarbons thermal cracking: Reactive force field and density functional calculations. Computational and Theoretical Chemistry, 2008, 852, 62-70.	1.5	16
129	The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. Theoretical Chemistry Accounts, 2008, 120, 215-241.	0.5	23,928
130	Strength of Câ€“H Bonds at Nitrogen Î± â€Position:Implication for Metabolic Stability of Nitrogenâ€containing Drug Molecules. Chinese Journal of Chemistry, 2008, 26, 787-793.	2.6	8
131	A DFTâ€Based Investigation of Hydrogen Abstraction Reactions from Methylated Polycyclic Aromatic Hydrocarbons. ChemPhysChem, 2008, 9, 2349-2358.	1.0	27
132	Theoretical Description of Substituent Effects in Electrophilic Aromatic Substitution Reactions. European Journal of Organic Chemistry, 2008, 2008, 5928-5935.	1.2	10
133	Neutral MÃ¶bius 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
134	Rearrangement and decomposition of (CH3)3M+ (M=Si, Ge, Sn) ions: A DFT study. Journal of Organometallic Chemistry, 2008, 693, 2856-2862.	0.8	9
135	Analytical representation of the Beckeâ€“Roussel exchange functional. Chemical Physics Letters, 2008, 455, 103-109.	1.2	25
136	The covalently bound HNC dimer ion HN C C NH+ has a kinetically stable neutral counterpart. Chemical Physics Letters, 2008, 462, 152-157.	1.2	20
137	Theoretical calculations of energetics, structures, and rate constants for the H+CH3OH hydrogen abstraction reactions. Chemical Physics Letters, 2008, 463, 33-37.	1.2	36
138	Sr2+-neutral molecules interactions: An assessment of theoretical procedures. Chemical Physics Letters, 2008, 464, 240-244.	1.2	10
139	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. Chemical Physics Letters, 2008, 465, 226-229.	1.2	96
140	Modelling the interaction of molecular hydrogen with lithium-doped hydrogen storage materials. Chemical Physics Letters, 2008, 467, 126-130.	1.2	60
141	A comparative post-Hartreeâ€“Fock and density functional theory study of monochalcogenide diatomic molecules. Computational and Theoretical Chemistry, 2008, 863, 79-83.	1.5	7
142	Density Functionals with Broad Applicability in Chemistry. Accounts of Chemical Research, 2008, 41, 157-167.	7.6	6,193

#	Article	IF	Citations
143	Orbital-dependent density functionals: Theory and applications. Reviews of Modern Physics, 2008, 80, 3-60.	16.4	1,069
144	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes:â€‰ Conventional versus Long-Range Hybrids. Journal of Chemical Theory and Computation, 2008, 4, 123-135.	2.3	766
145	Implementation and Performance of DFT-D with Respect to Basis Set and Functional for Study of Dispersion Interactions in Nanoscale Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2008, 4, 2030-2048.	2.3	161
146	Highly Accurate First-Principles Benchmark Data Sets for the Parametrization and Validation of Density Functional and Other Approximate Methods. Derivation of a Robust, Generally Applicable, Double-Hybrid Functional for Thermochemistry and Thermochemical Kinetics. Journal of Physical Chemistry A, 2008, 112, 12868-12886.	1.1	680
147	How Well Can New-Generation Density Functionals Describe the Energetics of Bond-Dissociation Reactions Producing Radicals?. Journal of Physical Chemistry A, 2008, 112, 1095-1099.	1.1	359
148	Double-Hybrid Functionals for Thermochemical Kinetics. Journal of Physical Chemistry A, 2008, 112, 3-8.	1.1	213
149	Consequences of Spin Contamination in Unrestricted Calculations on Open-Shell Species: Effect of Hartreeâ"Fock and MÃ¸llerâ"Plesset Contributions in Hybrid and Double-Hybrid Density Functional Theory Approaches. Journal of Physical Chemistry A, 2008, 112, 13225-13230.	1.1	137
150	Accurate Benchmark Calculation of the Reaction Barrier Height for Hydrogen Abstraction by the Hydroperoxyl Radical from Methane. Implications for C_nH_{2n+2} where n = 2 â† 4. Journal of Physical Chemistry A, 2008, 112, 7047-7054.	1.1	105
151	An Intrinsic Radical Stability Scale from the Perspective of Bond Dissociation Enthalpies: A Companion to Radical Electrophilicities. Journal of Organic Chemistry, 2008, 73, 9109-9120.	1.7	50
152	Through-space interactions between parallel-offset arenes at the van der Waals distance: 1,8-diarylbiphenylene syntheses, structure and QM computations. Physical Chemistry Chemical Physics, 2008, 10, 2686.	1.3	85
153	Benchmark calculations on the adiabatic ionization potentials of Mâ€“NH3â€ˆ(M=Na,Al,Ga,In,Cu,Ag). Journal of Chemical Physics, 2008, 128, 154301.	1.2	16
154	Exploring the Limit of Accuracy of the Global Hybrid Meta Density Functional for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2008, 4, 1849-1868.	2.3	956
155	Applicability of hybrid density functional theory methods to calculation of molecular hyperpolarizability. Journal of Chemical Physics, 2008, 129, 044109.	1.2	150
156	Systematic optimization of long-range corrected hybrid density functionals. Journal of Chemical Physics, 2008, 128, 084106.	1.2	2,890
157	Using elementary reactions to model growth processes of polyaromatic hydrocarbons under pyrolysis conditions of light feedstocks. Molecular Simulation, 2008, 34, 193-199.	0.9	11
158	Are the Radical Centers in Peptide Radical Cations Mobile? The Generation, Tautomerism, and Dissociation of Isomeric Î±-Carbon-Centered Triglycine Radical Cations in the Gas Phase. Journal of the American Chemical Society, 2008, 130, 7862-7872.	6.6	83
159	Potential energy curves and electronic structure of 3d transition metal hydrides and their cations. Journal of Chemical Physics, 2008, 129, 214302.	1.2	32
160	Theoretical Investigation of the Electronic Asymmetry of the Special Pair Cation Radical in the Photosynthetic Type-II Reaction Center. Journal of Physical Chemistry B, 2008, 112, 13923-13933.	1.2	25

#	Article	IF	Citations
161	Multicoefficient Density Functional Theory (MCâ^'DFT). Journal of Physical Chemistry A, 2008, 112, 1064-1070.	1.1	7
162	Benchmark Data for Interactions in Zeolite Model Complexes and Their Use for Assessment and Validation of Electronic Structure Methods. Journal of Physical Chemistry C, 2008, 112, 6860-6868.	1.5	157
163	G3//BMK and Its Application to Calculation of Bond Dissociation Enthalpies. Journal of Chemical Theory and Computation, 2008, 4, 1324-1331.	2.3	23
164	Semiempirical Double-Hybrid Density Functional with Improved Description of Long-Range Correlation. Journal of Physical Chemistry A, 2008, 112, 2702-2712.	1.1	123
165	Claisen Rearrangement of Aliphatic Allyl Vinyl Ethers in the Presence of Copper(II) Bisoxazoline. Journal of Organic Chemistry, 2008, 73, 4800-4809.	1.7	13
166	Theoretical Thermodynamics for Large Molecules: Walking the Thin Line between Accuracy and Computational Cost. Accounts of Chemical Research, 2008, 41, 569-579.	7.6	329
167	Bond Dissociation Enthalpies of Large Aromatic Carbon-Centered Radicals. Journal of Physical Chemistry A, 2008, 112, 13566-13573.	1.1	35
168	A new parameter-free correlation functional based on an average atomic reduced density gradient analysis. Journal of Chemical Physics, 2008, 128, 034101.	1.2	56
169	Equilibrium structure of the hydrogen bonded dimer H₂O Â·Â·Â· HF1. Molecular Physics, 2008, 106, 1249-1256.	0.8	13
170	Oscillations in meta-generalized-gradient approximation potential energy surfaces for dispersion-bound complexes. Journal of Chemical Physics, 2009, 131, 034111.	1.2	153
172	Post-CCSD(T) ab Initio Thermochemistry of Halogen Oxides and Related Hydrides XOX, XOOX, 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
173	Constrained density functional theory based configuration interaction improves the prediction of reaction barrier heights. Journal of Chemical Physics, 2009, 130, 034109.	1.2	79
174	Infrared multiphoton electron detachment spectroscopy of C762â^'. Journal of Chemical Physics, 2009, 131, 124306.	1.2	10
175	On the Reaction of Glycerol Dehydratase with Butâ€3â€eneâ€1,2â€diol. Chemistry - A European Journal, 2009, 15, 4865-4873.	1.7	10
176	The Variable Strength of the Sulfurâ€"Sulfur Bond: 78 to 41 kcal â€" G3, CBSâ€Q, and DFT Bond Energies of Sulfur (S₈) and Disulfanes XSSX (X = H, F, Cl, CH₃, CN, NH₂, OH,) Tj ETQq0 0 0 rgBT /Overlock 1	1.0	27
177	Evaluation of exchangeâ€correlation functionals for timeâ€dependent density functional theory calculations on metal complexes. Journal of Computational Chemistry, 2010, 31, 1008-1014.	1.5	27
178	How the choice of a computational model could rule the chemical interpretation: The Ni(II) catalyzed ethylene dimerization as a case study. Journal of Computational Chemistry, 2010, 31, 1053-1062.	1.5	8
179	Barrier heights for Hâ€atom abstraction by HÈ®₂ from nâ€butanolâ€"A simple yet exacting test for model chemistries?. Journal of Computational Chemistry, 2010, 31, 1236-1248.	1.5	80

#	Article	IF	Citations
180	Gas-phase acidity, bond dissociation energy and enthalpy of formation of fluorine-substituted benzenes: A theoretical study. Journal of Fluorine Chemistry, 2009, 130, 621-628.	0.9	20
181	Addition of sulfenic acids to monosubstituted acetylenes: a theoretical and experimental study. Journal of Physical Organic Chemistry, 2009, 22, 1048-1057.	0.9	23
182	TD-DFT benchmark for indigoÃ¯d dyes. Computational and Theoretical Chemistry, 2009, 914, 100-105.	1.5	37
183	Computational search for nonlinear optical materials: are polarization functions important in the hyperpolarizability predictions of molecules and aggregates?. Mendeleev Communications, 2009, 19, 311-313.	0.6	40
184	Density functional theory study of the mechanism for Ni(NHC)2 catalyzed dehydrogenation of ammoniaâ€“borane for chemical hydrogen storage. Journal of Organometallic Chemistry, 2009, 694, 2831-2838.	0.8	35
185	DFT study of molybdenaâ€“silica system â€“ A selection of density functionals based on their performance in thermochemistry of molybdenum compounds. Chemical Physics Letters, 2009, 469, 140-144.	1.2	30
186	O-atom transfer reaction from N2O to CO: A theoretical investigation. Chemical Physics Letters, 2009, 475, 202-207.	1.2	12
187	What is the energy barrier for H2 dissociation on Group 13 sub-nanosized metal cluster to form dihydride? Density functional dependence study. Chemical Physics Letters, 2009, 482, 15-19.	1.2	8
188	Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. Journal of Chemical Theory and Computation, 2009, 5, 2420-2435.	2.3	942
189	â€œMindlessâ€•DFT Benchmarking. Journal of Chemical Theory and Computation, 2009, 5, 993-1003.	2.3	215
190	Computation of accurate excitation energies for large organic molecules with double-hybrid density functionals. Physical Chemistry Chemical Physics, 2009, 11, 4611.	1.3	252
191	Superbasicity of a Bis-guanidino Compound with a Flexible Linker: A Theoretical and Experimental Study. Journal of the American Chemical Society, 2009, 131, 16858-16868.	6.6	79
192	Time-Dependent Density Functional Theory Study of the Electronic Excitation Spectra of Chlorophyllide a and Pheophorbide a in Solvents. Journal of Physical Chemistry B, 2009, 113, 4817-4825.	1.2	29
193	Accurate Thermochemistry for Transition Metal Oxide Clusters. Journal of Physical Chemistry A, 2009, 113, 7861-7877.	1.1	156
194	Electronic Properties of a New Two-Photon Absorbing Fluorene Derivative: The Role of Hartreeâ€“Fock Exchange in the Density Functional Theory Design of Improved Nonlinear Chromophores. Journal of Physical Chemistry C, 2009, 113, 20719-20724.	1.5	49
195	Ion-Pair Binding Energies of Ionic Liquids: Can DFT Compete with Ab Initio-Based Methods?. Journal of Physical Chemistry A, 2009, 113, 7064-7072.	1.1	163
196	Hydrogen Bonding Described Using Dispersion-Corrected Density Functional Theory. Journal of Physical Chemistry B, 2009, 113, 4726-4732.	1.2	60
197	Performance of Ab Initio and Density Functional Methods for Conformational Equilibria of C_nH_{2n+2} Alkane Isomers (n = 4â^'8). Journal of Physical Chemistry A, 2009, 113, 11974-11983.	1.1	156

#	Article	IF	Citations
198	Ultrafast Dynamics of Isolated Phenylcarbenes Followed by Femtosecond Time-Resolved Velocity Map Imaging. Journal of Physical Chemistry A, 2009, 113, 3041-3050.	1.1	21
199	Theoretical Study of Photochromic Compounds. 1. Bond Length Alternation and Absorption Spectra for the Open and Closed Forms of 29 Diarylethene Derivatives. Journal of Physical Chemistry A, 2009, 113, 8409-8414.	1.1	61
200	H2 Activation by a (PNP)Ir(C6H5) Complex via the Dearomatization/Aromatization Process of the PNP Ligand: A Computational Study. Inorganic Chemistry, 2009, 48, 10257-10263.	1.9	43
201	DFT Study on the Propagation Kinetics of Free-Radical Polymerization of Î±-Substituted Acrylates. Macromolecules, 2009, 42, 3033-3041.	2.2	72
202	Electronic Hyperpolarizabilities for Donorâ^'Acceptor Molecules with Long Conjugated Bridges: Calculations versus Experiment. Journal of Physical Chemistry A, 2009, 113, 10994-11001.	1.1	129
203	Benchmark Data for Noncovalent Interactions in HCOOHÂ·Â·Â·Benzene Complexes and Their Use for Validation of Density Functionals. Journal of Chemical Theory and Computation, 2009, 5, 2726-2733.	2.3	30
204	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. Journal of Physical Chemistry A, 2009, 113, 5786-5799.	1.1	114
205	H/Br Exchange in BBr₃ by HSiR₃ (R = H, CH₃,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 4 Barrier. Journal of Physical Chemistry A, 2009, 113, 12035-12043.	1.1	12
206	Rate Constant Rules for the Automated Generation of Gas-Phase Reaction Mechanisms. Journal of Physical Chemistry A, 2009, 113, 367-380.	1.1	95
207	Levofloxacin ozonation in water: Rate determining process parameters and reaction pathway elucidation. Chemosphere, 2009, 76, 683-689.	4.2	109
208	Cleavage of Carbon Dioxide by an Iridium-Supported Fischer Carbene. A DFT Investigation. Journal of the American Chemical Society, 2009, 131, 5800-5808.	6.6	43
209	Density functional theory for transition metals and transition metal chemistry. Physical Chemistry Chemical Physics, 2009, 11, 10757.	1.3	1,431
210	Photochemistry of 2-Nitrobenzylidene Acetals. Journal of Organic Chemistry, 2009, 74, 8647-8658.	1.7	22
211	Effects of Hydration on the Proton Transfer Mechanism in the Adenineâ^'Thymine Base Pair. Journal of Physical Chemistry A, 2009, 113, 7892-7898.	1.1	71
212	The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-821.	2.3	462
213	Ionization Energies of Aqueous Nucleic Acids: Photoelectron Spectroscopy of Pyrimidine Nucleosides and ab Initio Calculations. Journal of the American Chemical Society, 2009, 131, 6460-6467.	6.6	134
214	Spectral Properties of Spirooxazine Photochromes: TD-DFT Insights. Journal of Physical Chemistry A, 2009, 113, 13004-13012.	1.1	34
215	Examination of DFT and TDDFT Methods II. Journal of Physical Chemistry A, 2009, 113, 10873-10879.	1.1	19

#	Article	IF	Citations
216	Competing Mechanistic Channels in the Oxidation of Aldehydes by Ozone. Journal of Organic Chemistry, 2009, 74, 2108-2113.	1.7	36
217	Can short-range hybrids describe long-range-dependent properties?. Journal of Chemical Physics, 2009, 131, 044108.	1.2	426
218	Theoretical Prediction of the Nâˆ'H and Oâˆ'H Bonds Cleavage Catalyzed by the Single-Walled Silicon Carbide Nanotube. Journal of Physical Chemistry C, 2009, 113, 16736-16740.	1.5	39
219	Benchmark Thermochemistry of the C_nH_{2n+2} Alkane Isomers (n = 2â^'8) and Performance of DFT and Composite Ab Initio Methods for Dispersion-Driven Isomeric Equilibria. Journal of Physical Chemistry A, 2009, 113, 8434-8447.	1.1	128
220	Atomization energies of the carbon clusters C_n (n= 2â^'10) revisited by means of W4 theory as well as density functional, Gn, and CBS methods. Molecular Physics, 2009, 107, 977-990.	0.8	41
221	Excited-state lifetime of propadienylidene, l-C3H2. Physical Chemistry Chemical Physics, 2009, 11, 5353.	1.3	15
222	A theoretical study of the rearrangement processes of energized CCCB and CCCAl. Physical Chemistry Chemical Physics, 2009, 11, 7553.	1.3	10
223	Gas-phase reaction between calcium monocation and fluoromethane: Analysis of the potential energy hypersurface and kinetics calculations. Journal of Chemical Physics, 2009, 131, 144309.	1.2	8
224	Neural network approach to quantum-chemistry data: Accurate prediction of density functional theory energies. Journal of Chemical Physics, 2009, 131, 074104.	1.2	144
225	Hydrotrioxides Rather than Cyclic Tetraoxides (Tetraoxolanes) as the Primary Reaction Intermediates in the Low-Temperature Ozonation of Aldehydes. The Case of Benzaldehyde. Journal of Organic Chemistry, 2009, 74, 96-101.	1.7	14
226	Hydroxyl Radical Initiated Oxidation of s-Triazine: Hydrogen Abstraction Is Faster than Hydroxyl Addition. Journal of Physical Chemistry A, 2009, 113, 8596-8606.	1.1	28
227	Calculating Accurate Proton Chemical Shifts of Organic Molecules with Density Functional Methods and Modest Basis Sets. Journal of Organic Chemistry, 2009, 74, 4017-4023.	1.7	276
228	Synthesis, X-ray crystal structures, and computational studies of 1,1â€²-bridged 4,4â€²-diaryl-2,2â€²-bibenzimidazoles: building blocks for supramolecular structures. Organic and Biomolecular Chemistry, 2009, 7, 2347.	1.5	9
229	Performance of the major semiempirical, ab initio, and density functional theory methods in evaluating isomerization enthalpies for linear to branched heptanes. Nature Precedings, 2010, , .	0.1	6
230	Basis set effects on the hyperpolarizability of CHCl3: Gaussian-type orbitals, numerical basis sets and real-space grids. Journal of Chemical Physics, 2010, 133, 034111.	1.2	46
231	A universal approach for continuum solvent pK a calculations: are we there yet?. Theoretical Chemistry Accounts, 2010, 125, 3-21.	0.5	408
232	Computational methods for analysis of an unsaturated carbocycle: heptafulvene. Theoretical Chemistry Accounts, 2010, 126, 55-73.	0.5	8
233	Theoretical study of the competitive decomposition and isomerization of 1-hexyl radical. Theoretical Chemistry Accounts, 2010, 126, 87-98.	0.5	16

#	Article	IF	Citations
234	The electronic properties of a homoleptic bisphosphine Cu(I) complex: A joint theoretical and experimental insight. Computational and Theoretical Chemistry, 2010, 962, 7-14.	1.5	16
235	The electronic spectrum of AgBr2: Ab initio benchmark vs. DFT calculations on the lowest ligand-field states including spinâ€“orbit effects. Journal of Molecular Spectroscopy, 2010, 263, 166-173.	0.4	5
236	Density-functional calculations for large systems: Can GGA functionals Be competitive with hybrid functionals?. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 163-168.	2.2	10
237	Theoretical study on redox potentials of organic radicals in different solvents. Research on Chemical Intermediates, 2010, 36, 1003-1019.	1.3	8
238	The X1s Method for Accurate Bond Dissociation Energies. ChemPhysChem, 2010, 11, 2561-2567.	1.0	24
239	Firstâ€Principles Prediction of Nucleophilicity Parameters for Ï€ Nucleophiles: Implications for Mechanistic Origin of Mayrâ€™s Equation. Chemistry - A European Journal, 2010, 16, 2586-2598.	1.7	41
240	Regiospecific nucleophilic substitution in 2,3,4,5,6-pentafluorobiphenyl as model compound for supramolecular systems. Theoretical study of transition states and energy profiles, evidence for tetrahedral SN2 mechanism. Journal of Fluorine Chemistry, 2010, 131, 1327-1337.	0.9	43
241	Phosphate ester hydrolysis of biologically relevant molecules by cerium oxide nanoparticles. Nanomedicine: Nanotechnology, Biology, and Medicine, 2010, 6, 738-744.	1.7	171
242	Hydrogen abstraction from biphenyl, acenaphthylene, naphthalene and phenanthrene by atomic hydrogen and methyl radical: DFT and G3(MP2)-RAD data. Computational and Theoretical Chemistry, 2010, 940, 115-118.	1.5	26
243	Theoretical study of the molecular properties and the formation kinetics of the FS(O2)OCO radical. Chemical Physics Letters, 2010, 490, 127-131.	1.2	1
244	Hybrid DFT and hyper-GGA DFT studies of the CO adsorption on Pt nanoclusters: Effects of the cluster size and better CO LUMO description. Chemical Physics Letters, 2010, 492, 98-102.	1.2	24
245	Assessment of density functional methods for the study of olefin metathesis catalysed by ruthenium alkylidene complexes. Chemical Physics Letters, 2010, 493, 273-278.	1.2	60
246	Theoretical and experimental studies on stability of the Câ€ON bond in new ketone functionalized Nâ€alkoxyamines. Journal of Physical Organic Chemistry, 2010, 23, 1146-1154.	0.9	8
247	QUANTUM-CHEMICAL PREDICTION OF FORMATION ENTHALPY OF CYCLOALKANE. Journal of Theoretical and Computational Chemistry, 2010, 09, 155-166.	1.8	0
248	XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. Journal of Chemical Physics, 2010, 132, 194105.	1.2	40
249	Tests of the RPBE, revPBE, Ï„-HCTHhyb, Ï‰B97X-D, and MOHLYP density functional approximations and 29 others against representative databases for diverse bond energies and barrier heights in catalysis. Journal of Chemical Physics, 2010, 132, 164117.	1.2	206
251	THEORETICAL STUDY ON OXYGENâ€“OXYGEN HOMOLYTIC BOND DISSOCIATION ENTHALPIES OF PEROXIDES. Journal of Theoretical and Computational Chemistry, 2010, 09, 625-635.	1.8	2
252	Predicting Rate Constants for Nucleophilic Reactions of Amines with Diarylcarbenium Ions Using an ONIOM Method. Chinese Journal of Chemical Physics, 2010, 23, 669-674.	0.6	2

#	Article	IF	Citations
253	Multilevel Computational Analysis of Fluorocarbon Polyatomic Deposition on Diamond. Journal of Physical Chemistry C, 2010, 114, 12535-12544.	1.5	2
254	Thermochemical Properties of exo-Tricyclo[5.2.1.0^{2,6}]decane (JP-10 Jet Fuel) and Derived Tricyclodecyl Radicals. Journal of Physical Chemistry A, 2010, 114, 9545-9553.	1.1	42
255	Factors Dictating Carbene Formation at (PNP)Ir. Organometallics, 2010, 29, 4239-4250.	1.1	16
256	Assessment of TD-DFT methods and of various spin scaled CIS(D) and CC2 versions for the treatment of low-lying valence excitations of large organic dyes. Journal of Chemical Physics, 2010, 132, .	1.2	313
257	Bridged Photochromic Diarylethenes Investigated by Ultrafast Absorption Spectroscopy: Evidence for Two Distinct Photocyclization Pathways. Journal of the American Chemical Society, 2010, 132, 7379-7390.	6.6	62
258	Extending the reliability and applicability of B3LYP. Chemical Communications, 2010, 46, 3057.	2.2	196
259	Absorption Spectra of Riboflavinâ€"A Difficult Case for Computational Chemistry. Journal of Physical Chemistry A, 2010, 114, 10234-10242.	1.1	25
260	Global Hybrid Functionals: A Look at the Engine under the Hood. Journal of Chemical Theory and Computation, 2010, 6, 3688-3703.	2.3	87
261	Accuracy of computational solvation free energies for neutral and ionic compounds: Dependence on level of theory and solvent model. Nature Precedings, 0, , .	0.1	12
262	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. Journal of Chemical Theory and Computation, 2010, 6, 2872-2887.	2.3	1,183
263	DFT Study on the Standard Electrode Potentials of Imidazole, Tetrathiafulvalene, and Tetrathiafulvaleneâ^'Imidazole. Journal of Physical Chemistry B, 2010, 114, 17092-17101.	1.2	19
264	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
265	Effects of London dispersion on the isomerization reactions of large organic molecules: a density functional benchmark study. Physical Chemistry Chemical Physics, 2010, 12, 6940.	1.3	123
266	Computational Strategies for Reactions of Aggregated and Solvated Organolithium Carbenoids. Journal of Physical Chemistry A, 2010, 114, 8423-8433.	1.1	28
267	Integration Grid Errors for Meta-GGA-Predicted Reaction Energies: Origin of Grid Errors for the M06 Suite of Functionals. Journal of Chemical Theory and Computation, 2010, 6, 395-404.	2.3	332
268	Assessment of DFT and DFT-D for Potential Energy Surfaces of Rare Gas Trimersâ€"Implementation and Analysis of Functionals and Extrapolation Procedures. Journal of Chemical Theory and Computation, 2010, 6, 1951-1965.	2.3	8
269	Mechanism of Water Splitting and Oxygenâ^'Oxygen Bond Formation by a Mononuclear Ruthenium Complex. Journal of the American Chemical Society, 2010, 132, 120-130.	6.6	133
270	Calculations of Alkane Energies Using Long-Range Corrected DFT Combined with Intramolecular van der Waals Correlation. Organic Letters, 2010, 12, 1440-1443.	2.4	59

#	Article	IF	Citations
271	Structures and Energetics of Unimolecular Thermal Degradation of Isopropyl Butanoate as a Model Biofuel: Density Functional Theory and Ab Initio Studies. Journal of Physical Chemistry A, 2010, 114, 7996-8002.	1.1	14
272	Unimolecular Î²-Hydroxyperoxy Radical Decomposition with OH Recycling in the Photochemical Oxidation of Isoprene. Environmental Science & Technology, 2010, 44, 250-256.	4.6	122
273	Toward an Accurate Modeling of the Waterâ^'Zeolite Interaction: Calibrating the DFT Approach. Journal of Physical Chemistry Letters, 2010, 1, 763-768.	2.1	12
274	A QM/QM Multilayer Composite Methodology: The ONIOM Correlation Consistent Composite Approach (ONIOM-ccCA). Journal of Physical Chemistry A, 2010, 114, 9394-9397.	1.1	17
275	Kinetics of hydrogen-transfer isomerizations of butoxyl radicals. Physical Chemistry Chemical Physics, 2010, 12, 7782.	1.3	151
276	Intramolecular Ï€â^'Ï€ Stacking Interactions in 2-Substituted N,N-Dibenzylaziridinium Ions and Their Regioselectivity in Nucleophilic Ring-Opening Reactions. Journal of Organic Chemistry, 2010, 75, 885-896.	1.7	66
277	Assessing the Performance of Density Functional Theory for the Electronic Structure of Metalâ^'Salens: The M06 Suite of Functionals and the d⁴-Metals. Journal of Physical Chemistry A, 2010, 114, 11714-11718.	1.1	35
278	A Theoretical Study of Brominated Porphycenes: Electronic Spectra and Intersystem Spinâ^'Orbit Coupling. Journal of Chemical Theory and Computation, 2010, 6, 3176-3189.	2.3	21
279	A DFT and ab Initio Benchmarking Study of Metalâ^'Alkane Interactions and the Activation of Carbonâ^'Hydrogen Bonds. Journal of Physical Chemistry A, 2010, 114, 1843-1851.	1.1	32
280	Challenges Posed to Bornyl Diphosphate Synthase: Diverging Reaction Mechanisms in Monoterpenes. Journal of the American Chemical Society, 2010, 132, 6349-6360.	6.6	97
281	A Highly Diastereoselective Synthesis of Î±-Hydroxy-Î²-amino Acid Derivatives via a Lewis Acid Catalyzed Three-Component Condensation Reaction. Journal of Organic Chemistry, 2010, 75, 7099-7106.	1.7	25
282	On the Free Radical Scavenging Capability of Carboxylated Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 6363-6370.	1.5	32
283	Formation Enthalpies of Ions: Routine Prediction Using Atom Equivalents. Journal of Chemical Theory and Computation, 2010, 6, 2126-2139.	2.3	4
284	Trends in Râ^'X Bond Dissociation Energies (Râ€¢ = Me, Et, i-Pr, t-Bu, Xâ€¢ = H, Me, Cl, OH). Journal of Chemical Theory and Computation, 2010, 6, 1462-1469.	2.3	39
285	Bond Dissociation Energies of Organophosphorus Compounds: an Assessment of Contemporary Ab Initio Procedures. Journal of Physical Chemistry A, 2010, 114, 2864-2873.	1.1	35
286	Comprehensive evaluation of medium and long range correlated density functionals in TD-DFT investigation of DNA bases and base pairs: gas phase and water solution study. Molecular Physics, 2010, 108, 3131-3146.	0.8	19
287	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. Journal of Chemical Theory and Computation, 2010, 6, 370-383.	2.3	202
288	DSD-BLYP: A General Purpose Double Hybrid Density Functional Including Spin Component Scaling and Dispersion Correction. Journal of Physical Chemistry C, 2010, 114, 20801-20808.	1.5	329

#	Article	IF	Citations
289	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. Journal of Chemical Theory and Computation, 2010, 6, 2071-2085.	2.3	383
290	Homogeneous Ni Catalysts for H2Oxidation and Production: An Assessment of Theoretical Methods, from Density Functional Theory to Post Hartreeâ^'Fock Correlated Wave-Function Theory. Journal of Physical Chemistry A, 2010, 114, 12716-12724.	1.1	44
291	Radical routes to interstellar glycolaldehyde. The possibility of stereoselectivity in gas-phase polymerization reactions involving CH2O and Ë™CH2OH. Organic and Biomolecular Chemistry, 2010, 8, 4757.	1.5	15
292	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. Physical Chemistry Chemical Physics, 2010, 12, 8016.	1.3	126
293	Theoretical Study of the Thermal Decomposition of Dimethyl Disulfide. Journal of Physical Chemistry A, 2010, 114, 10531-10549.	1.1	57
294	Kinetic and Mechanistic Study onp-Quinodimethane Formation in the Sulfinyl Precursor Route for the Polymerization of Poly(p-phenylenevinylene) (PPV). Macromolecules, 2010, 43, 7424-7433.	2.2	26
295	Prediction of Reliable Metalâ^'PH₃ Bond Energies for Ni, Pd, and Pt in the 0 and +2 Oxidation States. Inorganic Chemistry, 2010, 49, 5546-5553.	1.9	21
296	Analytic gradients for the combinedsr-DFT/lr-MP2 method: application to weakly bound systems. Molecular Physics, 2010, 108, 3373-3382.	0.8	8
297	On the SmCo Dimer: A Detailed Density Functional Theory Analysis. Journal of Physical Chemistry A, 2010, 114, 1897-1905.	1.1	1
298	Theoretical study on the mechanism of H₂activation mediated by two transition metal thiolate complexes: Homolytic for Ir, heterolytic for Rh. Dalton Transactions, 2010, 39, 857-863.	1.6	21
299	Combined experimental and theoretical investigation into Câ€“H activation of cyclic alkanes by Cpâ€²Rh(CO)2 (Cpâ€² = Î·5-C5H5 or Î·5-C5Me5). Dalton Transactions, 2011, 40, 1751.	1.6	18
300	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. International Reviews in Physical Chemistry, 2011, 30, 115-160.	0.9	116
301	Dissociation of energy selected Sn(CH3)4+, Sn(CH3)3Cl+, and Sn(CH3)3Br+ ions: evidence for isolated excited state dynamics. Physical Chemistry Chemical Physics, 2011, 13, 17791.	1.3	21
302	Thermal Câ^'H Bond Activation of Benzene, Toluene, and Methane with Cationic [M(X)(bipy)]+(M = Ni, Pd,) Tj ETQq1 1 0.784314 rgBT	1.1	46
303	Regression Formulas for Density Functional Theory Calculated ¹H and ¹³C NMR Chemical Shifts in Toluene-d₈. Journal of Physical Chemistry A, 2011, 115, 12364-12372.	1.1	50
304	Modeling Proton Transfer in Imidazole-like Dimers: A Density Functional Theory Study. Journal of Physical Chemistry A, 2011, 115, 2627-2634.	1.1	26
305	Ring-opening radical clock reactions: many density functionals have difficulty keeping time. Organic and Biomolecular Chemistry, 2011, 9, 3158.	1.5	5
306	Tuning the Laplaza-Cummins 3-coordinate M[N(R)Ph]3 catalyst to activate and cleave CO2. Dalton Transactions, 2011, 40, 5569.	1.6	12

#	Article	IF	Citations
307	On the performance of density functional schemes for computing the static dipole polarizability of 4d transition-metal monohalides. Molecular Physics, 2011, 109, 1439-1452.	0.8	6
308	Improved DFT Description of Intrastrand Cross-Link Formation by Inclusion of London Dispersion Corrections. Journal of Physical Chemistry B, 2011, 115, 15138-15144.	1.2	22
309	Molecular Structures, Acidâ"Base Properties, and Formation of Group 6 Transition Metal Hydroxides. Journal of Physical Chemistry C, 2011, 115, 8072-8103.	1.5	54
310	Insights into the Solvation and Mobility of the Hydroxyl Radical in Aqueous Solution. Journal of Chemical Theory and Computation, 2011, 7, 3725-3732.	2.3	28
311	High-level direct-dynamics variational transition state theory calculations including multidimensional tunneling of the thermal rate constants, branching ratios, and kinetic isotope effects of the hydrogen abstraction reactions from methanol by atomic hydrogen. Journal of Chemical Physics, 2011, 134, 094302.	1.2	66
312	Theoretical Thermochemistry for Organic Molecules: Development of the Generalized Connectivity-Based Hierarchy. Journal of Chemical Theory and Computation, 2011, 7, 2094-2103.	2.3	77
313	Theoretical Study of Photochromic Compounds: Part 3. Prediction of Thermal Stability. Journal of Physical Chemistry C, 2011, 115, 10292-10297.	1.5	55
314	How Fast Do Microhydrated Al Clusters React: A Theoretical Study. Journal of Physical Chemistry C, 2011, 115, 24849-24857.	1.5	19
315	Assessment of TD-DFT and CC2 Methods for the Calculation of Resonance Raman Intensities: Application to o-Nitrophenol. Journal of Chemical Theory and Computation, 2011, 7, 1082-1089.	2.3	34
316	Carbonâ€"Bromine Bond Formation through a Nickel-Centered Spin-Crossing Mechanism. Organometallics, 2011, 30, 6365-6371.	1.1	19
317	Thermal Decomposition of 2-Butanol as a Potential Nonfossil Fuel: A Computational Study. Journal of Physical Chemistry A, 2011, 115, 2837-2846.	1.1	36
318	G4(MP2)-6X: A Cost-Effective Improvement to G4(MP2). Journal of Chemical Theory and Computation, 2011, 7, 112-120.	2.3	145
319	Density Functional and Spinâ"Orbit Ab Initio Study of CF₃Br: Molecular Properties and Electronic Curve Crossing. Journal of Physical Chemistry A, 2011, 115, 1264-1271.	1.1	12
320	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
321	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
322	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
323	Optical Behavior of Conjugated Pt-Containing Polymetallaynes Exposed to Gamma-Ray Radiation Doses. Journal of Physical Chemistry B, 2011, 115, 8047-8053.	1.2	15
324	Impact of tunneling on hydrogen-migration of the n-propylperoxy radical. Physical Chemistry Chemical Physics, 2011, 13, 17969.	1.3	74

#	Article	IF	Citations
326	Oscillator Strength: How Does TDDFT Compare to EOM-CCSD?. Journal of Chemical Theory and Computation, 2011, 7, 456-466.	2.3	123
327	Accuracy of Density Functionals in the Prediction of Electronic Proton Affinities of Amino Acid Side Chains. Journal of Chemical Theory and Computation, 2011, 7, 3898-3908.	2.3	45
328	Thermodynamics of Dimethylarsinic Acid and Arsenate Interactions with Hydrated Iron-(Oxyhydr)oxide Clusters: DFT Calculations. Environmental Science & Technology, 2011, 45, 10438-10444.	4.6	27
329	Ionization of Purine Tautomers in Nucleobases, Nucleosides, and Nucleotides: From the Gas Phase to the Aqueous Environment. Journal of Physical Chemistry B, 2011, 115, 1294-1305.	1.2	71
330	Ab initio and DFT studies of the spinâ€“orbit and spinâ€“spin contributions to the zero-field splitting tensors of triplet nitrenes with aryl scaffolds. Physical Chemistry Chemical Physics, 2011, 13, 6970.	1.3	44
331	Evaluating the Performance of DFT Functionals in Assessing the Interaction Energy and Ground-State Charge Transfer of Donor/Acceptor Complexes: Tetrathiafulvaleneâ^'Tetracyanoquinodimethane (TTFâ^'TCNQ) as a Model Case. Journal of Chemical Theory and Computation, 2011, 7, 602-609.	2.3	143
332	A DFT study of substituent effects in corannulene dimers. Physical Chemistry Chemical Physics, 2011, 13, 21139.	1.3	48
333	Computational Tests of Models for Kinetic Parameters of Unimolecular Reactions of Organophosphorus and Organosulfur Compounds. Journal of Physical Chemistry A, 2011, 115, 14143-14152.	1.1	6
334	Evaluation of the Nonlinear Optical Properties for Annulenes with HÃ¼ckel and MÃ¶bius Topologies. Journal of Chemical Theory and Computation, 2011, 7, 3935-3943.	2.3	86
335	Magnetic Coupling in Transition-Metal Binuclear Complexes by Spin-Flip Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2011, 7, 3523-3531.	2.3	52
336	Obtaining Good Performance With Triple-Î¶-Type Basis Sets in Double-Hybrid Density Functional Theory Procedures. Journal of Chemical Theory and Computation, 2011, 7, 2852-2863.	2.3	59
337	PO bond dissociation enthalpies: High-level ab initio and DFT study. Computational and Theoretical Chemistry, 2011, 968, 1-7.	1.1	9
338	Electronic structure, vibrational spectra and 1H NMR of halide ion (Fâ^', Clâ^' and Brâ^') encapsulated bambus[6]uril from density functional theory. Computational and Theoretical Chemistry, 2011, 976, 76-82.	1.1	16
339	A comparison of density functional theory (DFT) methods for estimating the singletâ€“triplet (S0â€“T1) excitation energies of benzene and polyacenes. Computational and Theoretical Chemistry, 2011, 976, 105-112.	1.1	36
340	Accurate prediction of experimental free energy of activation barriers for the aliphatic-Claisen rearrangement through DFT calculations. Computational and Theoretical Chemistry, 2011, 976, 167-182.	1.1	16
341	Thermodynamic and kinetic stability of magnesium dication solvated by tetramethylethylenediamine. Computational and Theoretical Chemistry, 2011, 978, 104-109.	1.1	4
342	DFT characterization of the first step of methyl acrylate polymerization: Performance of modern functionals in the complete basis limit. Computational and Theoretical Chemistry, 2011, 978, 88-97.	1.1	10
343	Oxidation of Zincâ€“Thiolate Complexes of Biological Interest by Hydrogen Peroxide: A Theoretical Study. Inorganic Chemistry, 2011, 50, 5407-5416.	1.9	25

#	Article	IF	Citations
344	Validation of electronic structure methods for isomerization reactions of large organic molecules. Physical Chemistry Chemical Physics, 2011, 13, 13683.	1.3	78
345	How reliable are DFT transition structures? Comparison of GGA, hybrid-meta-GGA and meta-GGA functionals. Organic and Biomolecular Chemistry, 2011, 9, 689-700.	1.5	212
346	Stereoselective Synthesis of cis-3,4-Disubstituted Piperidines through Ring Transformation of 2-(2-Mesyloxyethyl)azetidines. Journal of Organic Chemistry, 2011, 76, 8364-8375.	1.7	33
347	Benchmark results for empirical post-GGA functionals: Difficult exchange problems and independent tests. Physical Chemistry Chemical Physics, 2011, 13, 19325.	1.3	83
348	Reactivity of Activated versus Nonactivated 2-(Bromomethyl)aziridines with respect to Sodium Methoxide: A Combined Computational and Experimental Study. Journal of Organic Chemistry, 2011, 76, 8698-8709.	1.7	17
349	An examination of density functional theories on isomerization energy calculations of organic molecules. Theoretical Chemistry Accounts, 2011, 130, 851-857.	0.5	24
350	Origins of the diastereoselectivity in hydrogen bonding directed Dielsâ€“Alder reactions of chiral dienes with achiral dienophiles: a computational study. Organic and Biomolecular Chemistry, 2011, 9, 8079.	1.5	18
351	Semiempirical, Hartree-Fock, density functional, and second order Moller-Plesset perturbation theory methods do not accurately predict ionization energies and electron affinities of short- through long-chain [n]acenes. Nature Precedings, 2011, , .	0.1	1
352	The Contribution of Molecular Modeling to the Knowledge of Pesticides. , 2011, , .		0
353	Seeking for parameter-free double-hybrid functionals: The PBE0-DH model. Journal of Chemical Physics, 2011, 135, 024106.	1.2	226
354	Controlling the tacticity in the polymerization of N-isopropylacrylamide: A computational study. Polymer, 2011, 52, 5503-5512.	1.8	20
355	Photoinduced intramolecular charge transfer process of betaine pyridinium: A theoretical spectroscopic study. Chemical Physics Letters, 2011, 515, 42-48.	1.2	13
356	Accurate singlet and triplet excitation energies using the Localized Hartreeâ€“Fock Kohnâ€“Sham potential. Chemical Physics, 2011, 391, 19-26.	0.9	13
357	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. Physical Chemistry Chemical Physics, 2011, 13, 6670.	1.3	1,627
358	Unexpected Direct Reduction Mechanism for Hydrogenation of Ketones Catalyzed by Iron PNP Pincer Complexes. Inorganic Chemistry, 2011, 50, 12836-12843.	1.9	71
359	UV Photolysis of ClOOCl and the Ozone Hole. Chemistry - an Asian Journal, 2011, 6, 1664-1678.	1.7	14
360	Approximations to complete basis set-extrapolated, highly correlated non-covalent interaction energies. Journal of Chemical Physics, 2011, 135, 134318.	1.2	81
361	Key Building Block of Photoresponsive Biomimetic Systems. Journal of Physical Chemistry B, 2011, 115, 1232-1242.	1.2	6

#	Article	IF	Citations
362	How Well Can Modern Density Functionals Predict Internuclear Distances at Transition States?. Journal of Chemical Theory and Computation, 2011, 7, 1667-1676.	2.3	156
363	Valence and spin situations in isomeric [(bpy)Ru(Qâ€²)2]n (Qâ€² =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 707 Td (3,5-di-tert Transactions, 2011, 40, 8377.	1.6	37
364	Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. Physical Chemistry Chemical Physics, 2011, 13, 16987.	1.3	301
365	Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. Journal of Physical Chemistry Letters, 2011, 2, 2810-2817.	2.1	864
366	Theoretical study of substituent and solvent effects on the thermodynamics for cis/trans isomerization and intramolecular rearrangements of 2,2â€²-diphenoquinones. Structural Chemistry, 2011, 22, 615-625.	1.0	5
367	Computational characterization of sodium selenite using density functional theory. Journal of Molecular Modeling, 2011, 17, 701-708.	0.8	1
368	Assessment of the Ï‰B97 family for excited-state calculations. Theoretical Chemistry Accounts, 2011, 128, 127-136.	0.5	132
369	Hydrogen abstraction reactions of OH radicals with CF2ClCClXH (XÂ=ÂF, Cl) and CFCl2CClXH (XÂ=ÂF, Cl): a mechanistic and kinetic study. Theoretical Chemistry Accounts, 2011, 129, 73-84.	0.5	4
370	An examination of density functionals on aldol, Mannich and Î±-aminoxylation reaction enthalpy calculations. Theoretical Chemistry Accounts, 2011, 130, 153-160.	0.5	8
371	Assessment of theoretical procedures for hydrogen-atom abstraction by chlorine, and related reactions. Theoretical Chemistry Accounts, 2011, 130, 251-260.	0.5	37
372	Ground-state properties of the retinal molecule: from quantum mechanical to classical mechanical computations of retinal proteins. Theoretical Chemistry Accounts, 2011, 130, 1169-1183.	0.5	15
373	Applications and validations of the Minnesota density functionals. Chemical Physics Letters, 2011, 502, 1-13.	1.2	662
374	Intriguing Differences in the Gas-Phase Dissociation Behavior of Protonated and Deprotonated Gonyautoxin Epimers. Journal of the American Society for Mass Spectrometry, 2011, 22, 2011-20.	1.2	13
375	Cyclization tendencies in the free radical polymerization of allyl acrylate derivatives: A computational study. Journal of Polymer Science Part A, 2011, 49, 2474-2483.	2.5	8
376	A computational study of Cï£¿X (Xâ€‰=â€‰H, C, F, Cl) bond dissociation enthalpies (BDEs) in polyhalogenated methanes and ethanes. Journal of Physical Organic Chemistry, 2011, 24, 65-73.	0.9	18
377	Electron correlation and the stability of substituted alkenes. Journal of Physical Organic Chemistry, 2011, 24, 1222-1228.	0.9	5
378	Density functional theory study of the structure and energetics of negatively charged oligopyrroles. International Journal of Quantum Chemistry, 2011, 111, 2295-2305.	1.0	56
379	Dissociation curves and binding energies of diatomic transition metal carbides from density functional theory. International Journal of Quantum Chemistry, 2011, 111, 4276-4287.	1.0	11

#	Article	IF	Citations
380	Irreversible Inhibition of Monoamine Oxidase B by the Antiparkinsonian Medicines Rasagiline and Selegiline: A Computational Study. European Journal of Organic Chemistry, 2011, 2011, 6419-6433.	1.2	32
381	Computational study of static first hyperpolarizability of donorâ€“acceptor substituted (E)â€benzaldehyde phenylhydrazone. Journal of Computational Chemistry, 2011, 32, 730-736.	1.5	28
382	Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. Journal of Computational Chemistry, 2011, 32, 1824-1838.	1.5	26
383	A semiempirical longâ€range corrected exchange correlation functional including a shortâ€range Gaussian attenuation (LCgauâ€B97). Journal of Computational Chemistry, 2011, 32, 3269-3275.	1.5	13
384	Different properties for poly(3,4â€ethylenedioxythiophene) films derived from single or multiple polymerization steps. Journal of Applied Polymer Science, 2011, 121, 1982-1991.	1.3	17
386	Hydration of Carbonyl Groups: The Labile H₃O⁺ Ion as an Intermediate Modulated by the Surrounding Water Molecules. Angewandte Chemie - International Edition, 2011, 50, 3266-3270.	7.2	28
387	Can Enantioselectivity be Computed in Enthalpic Barrierless Reactions? The Case of Cu^Iâ€Catalyzed Cyclopropanation of Alkenes. Chemistry - A European Journal, 2011, 17, 529-539.	1.7	14
388	Competitive Reactions of Organophosphorus Radicals on Coke Surfaces. Chemistry - A European Journal, 2011, 17, 12027-12036.	1.7	23
389	Imidazole to NHC Rearrangements at Molybdenum Centers: An Experimental and Theoretical Study. Chemistry - A European Journal, 2011, 17, 8584-8595.	1.7	38
390	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. Chemical Physics Letters, 2011, 510, 165-178.	1.2	353
391	Modeling reaction pathways of low energy particle deposition on thiophene via ab initio calculations. Chemical Physics Letters, 2011, 510, 197-201.	1.2	2
392	Chemically accurate and computationally-efficient time-dependent density functional theory (TDDFT) modeling of the UV/Vis spectra of Pechmann dyes and related compounds. Procedia Computer Science, 2011, 4, 1157-1166.	1.2	5
393	Domino Dielsâ€“Alder reactions of N-methoxyethyl-7-oxa-norbornadiene-2,3-dicarboximide: an elusive, highly reactive dienophile. Tetrahedron, 2011, 67, 1580-1588.	1.0	11
394	Density functional study of multiplicity-changing valence and Rydberg excitations of p-block elements: Delta self-consistent field, collinear spin-flip time-dependent density functional theory (DFT), and conventional time-dependent DFT. Journal of Chemical Physics, 2011, 135, 044118.	1.2	57
395	O - H Bond Dissociation Energies. Australian Journal of Chemistry, 2011, 64, 394.	0.5	20
396	Benchmark of density functional theory methods on the prediction of bond energies and bond distances of noble-gas containing molecules. Journal of Chemical Physics, 2011, 134, 244110.	1.2	52
397	Improving the Accuracy of Density Functional Theory (DFT) Calculation for Homolysis Bond Dissociation Energies of Y-NO Bond: Generalized Regression Neural Network Based on Grey Relational Analysis and Principal Component Analysis. International Journal of Molecular Sciences, 2011, 12, 2242-2261.	1.8	12
398	Long-range corrected hybrid meta-generalized-gradient approximations with dispersion corrections. Journal of Chemical Physics, 2012, 136, 154109.	1.2	101

#	Article	IF	Citations
399	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
400	SËO homolytic bond dissociation enthalpies in sulfones: high-level ab initio and DFT study. Journal of Sulfur Chemistry, 2012, 33, 541-559.	1.0	1
401	CHAMELEON GROUND STATE AND EXCITED STATES OF EDT-TTF-IM-F4TCNQ RADICAL DYAD IN DIFFERENT ENVIRONMENTS. Journal of Theoretical and Computational Chemistry, 2012, 11, 505-525.	1.8	6
402	Dual-Level Direct Dynamics Studies on the Hydrogen Abstraction Reactions of CH2CH3 - n Xn+HBr (X=Cl, Br and n=1, 2). Australian Journal of Chemistry, 2012, 65, 160.	0.5	0
403	TD-DFT Assessment of Functionals for Optical 0â€“0 Transitions in Solvated Dyes. Journal of Chemical Theory and Computation, 2012, 8, 2359-2372.	2.3	403
404	Tunneling in H loss from energy selected ethanol ions. Physical Chemistry Chemical Physics, 2012, 14, 16047.	1.3	33
405	O(³P) + CO₂ Collisions at Hyperthermal Energies: Dynamics of Nonreactive Scattering, Oxygen Isotope Exchange, and Oxygen-Atom Abstraction. Journal of Physical Chemistry A, 2012, 116, 64-84.	1.1	19
406	Performance of Gradient-Corrected and Hybrid Density Functional Theory: Role of the Underlying Local Density Approximation and the Gradient Correction. Journal of Chemical Theory and Computation, 2012, 8, 4899-4906.	2.3	16
407	M11-L: A Local Density Functional That Provides Improved Accuracy for Electronic Structure Calculations in Chemistry and Physics. Journal of Physical Chemistry Letters, 2012, 3, 117-124.	2.1	531
408	Reliable Quantum Chemical Prediction of the Localized/Delocalized Character of Organic Mixed-Valence Radical Anions. From Continuum Solvent Models to Direct-COSMO-RS. Journal of Chemical Theory and Computation, 2012, 8, 4189-4203.	2.3	83
409	A detailed test study of barrier heights for the HO2 + H2O + O3 reaction with various forms of multireference perturbation theory. Journal of Chemical Physics, 2012, 136, 114312.	1.2	10
410	Ligand Bond Energies in cis- and trans-[L-Pd(PH₃)₂Cl]⁺ Complexes from Coupled Cluster Theory (CCSD(T)) and Density Functional Theory. Inorganic Chemistry, 2012, 51, 13195-13203.	1.9	17
411	Unrestricted Prescriptions for Open-Shell Singlet Diradicals: Using Economical Ab Initio and Density Functional Theory to Calculate Singletâ€“Triplet Gaps and Bond Dissociation Curves. Journal of Physical Chemistry A, 2012, 116, 4922-4929.	1.1	42
412	Time-Dependent Density Functional Theory Assessment of UV Absorption of Benzoic Acid Derivatives. Journal of Physical Chemistry A, 2012, 116, 11870-11879.	1.1	55
414	A Chiral Dicationic [8]Circulenoid: Photochemical Origin and Facile Thermal Conversion into a Helicene Congener. Angewandte Chemie - International Edition, 2012, 51, 11972-11976.	7.2	21
415	S=O homolytic bond dissociation enthalpies in sulfoxides. Research on Chemical Intermediates, 2012, 38, 1791-1806.	1.3	4
416	Bipolarons and polaron pairs in oligopyrrole dications. Computational and Theoretical Chemistry, 2012, 993, 7-12.	1.1	9
417	Which Density Functional Is the Best in Computing Câ€“H Activation Energies by Pincer Complexes of Late Platinum Group Metals?. Journal of Chemical Theory and Computation, 2012, 8, 2991-2996.	2.3	40

#	Article	IF	Citations
418	Charge transport in poly-imidazole membranes: a fresh appraisal of the Grotthuss mechanism. Physical Chemistry Chemical Physics, 2012, 14, 10910.	1.3	29
419	Aza-boron-dipyrromethene dyes: TD-DFT benchmarks, spectral analysis and design of original near-IR structures. Physical Chemistry Chemical Physics, 2012, 14, 157-164.	1.3	100
420	Parameter-free correlation for a composition-based prediction of the dielectric constant of amorphous organosilicate materials. Molecular Simulation, 2012, 38, 1221-1233.	0.9	5
421	Assessment of Density Functional Theory in Predicting Structures and Free Energies of Reaction of Atmospheric Prenucleation Clusters. Journal of Chemical Theory and Computation, 2012, 8, 2071-2077.	2.3	168
422	Theoretical Studies of the O(³P) + C₂ Reaction at Hyperthermal Energies. Journal of Physical Chemistry C, 2012, 116, 26577-26585.	1.5	5
423	Predicting the Localized/Delocalized Character of Mixed-Valence Diquinone Radical Anions. Toward the Right Answer for the Right Reason. Journal of Physical Chemistry A, 2012, 116, 10629-10637.	1.1	50
424	W1X-1 and W1X-2: W1-Quality Accuracy with an Order of Magnitude Reduction in Computational Cost. Journal of Chemical Theory and Computation, 2012, 8, 4259-4269.	2.3	79
425	Inner-Sphere Activation, Outer-Sphere Catalysis: Theoretical Study on the Mechanism of Transfer Hydrogenation of Ketones Using Iron(II) PNNP Eneamido Complexes. Organometallics, 2012, 31, 7375-7385.	1.1	79
426	Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation. Physical Review B, 2012, 85, .	1.1	1,087
427	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
428	Infrared Multiple-Photon Dissociation Spectroscopy of Tripositive Ions: Lanthanumâ€“Tryptophan Complexes. Inorganic Chemistry, 2012, 51, 4707-4710.	1.9	12
429	Benchmark Database for Ylidic Bond Dissociation Energies and Its Use for Assessments of Electronic Structure Methods. Journal of Chemical Theory and Computation, 2012, 8, 2824-2834.	2.3	62
430	Free radical polymerization of ethyl methacrylate and ethyl Î±-hydroxy methacrylate: A computational approach to the propagation kinetics. Polymer, 2012, 53, 3211-3219.	1.8	18
431	The catalytic mechanism of mouse renin studied with QM/MM calculations. Physical Chemistry Chemical Physics, 2012, 14, 12605.	1.3	21
432	How Evenly Can Approximate Density Functionals Treat the Different Multiplicities and Ionization States of 4d Transition Metal Atoms?. Journal of Chemical Theory and Computation, 2012, 8, 4112-4126.	2.3	37
433	Unraveling the Reactions that Unravel Cellulose. Journal of Physical Chemistry A, 2012, 116, 7098-7106.	1.1	176
434	DFT and Proton Transfer Reactions: A Benchmark Study on Structure and Kinetics. Journal of Chemical Theory and Computation, 2012, 8, 3082-3088.	2.3	85
435	How Accurate Can a Local Coupled Cluster Approach Be in Computing the Activation Energies of Late-Transition-Metal-Catalyzed Reactions with Au, Pt, and Ir?. Journal of Chemical Theory and Computation, 2012, 8, 3119-3127.	2.3	60

#	Article	IF	Citations
436	Isomerization energies of tetrahedranes to 1,3-cyclobutadienes: A challenge for theoretical methods. Computational and Theoretical Chemistry, 2012, 979, 1-9.	1.1	8
437	Structure and electronic spectral property of coumarinâ€“chalcone hybrids: A comparative study using conventional and long-range corrected hybrid functionals. Computational and Theoretical Chemistry, 2012, 981, 90-99.	1.1	32
438	Singletâ€“triplet excitation energies of naphthyl cations: High level composite method calculations suggest a singlet ground state. Computational and Theoretical Chemistry, 2012, 983, 69-75.	1.1	9
439	Kinetic study of the formation of triphenylene from the condensation of C12H10+C6H5. Computational and Theoretical Chemistry, 2012, 985, 1-7.	1.1	13
440	Libxc: A library of exchange and correlation functionals for density functional theory. Computer Physics Communications, 2012, 183, 2272-2281.	3.0	419
441	Kinetic modeling for hydrogen-abstraction reaction of methylcyclohexane with the CH3 radical. Chemical Engineering Science, 2012, 79, 200-209.	1.9	5
442	Elusive Metal-Free Primary Amination of Arylboronic Acids: Synthetic Studies and Mechanism by Density Functional Theory. Journal of the American Chemical Society, 2012, 134, 18253-18256.	6.6	139
443	Solventâ€Catalyzed Ringâ€“Chainâ€“Ring Tautomerization in Axially Chiral Compounds. Chemistry - A European Journal, 2012, 18, 12725-12732.	1.7	14
444	Theoretical investigation of the structure and electronic absorption spectrum of a complex zinc bis-[8-(3,5-difluorophenylsulfanylamino)quinolinate]. Optics and Spectroscopy (English Translation of) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.7	12
445	Ab initio quantum chemical and ReaxFF-based study of the intramolecular iminiumâ€“enamine conversion in a proline-catalyzed reaction. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	9
447	Benchmark Ab Initio Calculations of the Barrier Height and Transition-State Geometry for Hydrogen Abstraction from a Phenolic Antioxidant by a Peroxy Radical and Its Use to Assess the Performance of Density Functionals. Journal of Physical Chemistry Letters, 2012, 3, 2834-2839.	2.1	31
448	Approaches for Obtaining Accurate Rate Constants for Hydrogen Abstraction by a Chlorine Atom. Journal of Physical Chemistry A, 2012, 116, 3745-3752.	1.1	29
449	A computational study on the structures and energetics of isobutanol pyrolysis. Computational and Theoretical Chemistry, 2012, 997, 94-102.	1.1	9
450	Coupled Cluster and Density Functional Theory Calculations of Atomic Hydrogen Chemisorption on Pyrene and Coronene as Model Systems for Graphene Hydrogenation. Journal of Physical Chemistry A, 2012, 116, 7154-7160.	1.1	51
451	Transforming Anion Instability into Stability: Contrasting Photoionization of Three Protonation Forms of the Phosphate Ion upon Moving into Water. Journal of Physical Chemistry B, 2012, 116, 13254-13264.	1.2	48
452	Electron Transfer Triggers Fast Dimer/Monomer Switching of Pyridinium and Quinolinium Cations. Journal of Physical Chemistry C, 2012, 116, 3779-3786.	1.5	25
453	Mobility Mechanism of Hydroxyl Radicals in Aqueous Solution via Hydrogen Transfer. Journal of the American Chemical Society, 2012, 134, 532-538.	6.6	66
454	Complexes with a Single Metalâ€“Metal Bond as a Sensitive Probe of Quality of Exchange-Correlation Functionals. Journal of Chemical Theory and Computation, 2012, 8, 908-914.	2.3	54

#	Article	IF	Citations
455	On the Computation of Adiabatic Energies in Aza-Boron-Dipyrromethene Dyes. Journal of Chemical Theory and Computation, 2012, 8, 3303-3313.	2.3	102
456	Explicitly correlated benchmark calculations on C₈H₈ isomer energy separations: how accurate are DFT, double-hybrid, and composite ab initio procedures?. Molecular Physics, 2012, 110, 2477-2491.	0.8	63
457	Modern battery electrolytes: Ionâ€“ion interactions in Li+/Na+ conductors from DFT calculations. Physical Chemistry Chemical Physics, 2012, 14, 10774.	1.3	80
458	Density functional theory for the description of charge-transfer processes at TTF/TCNQ interfaces. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	15
459	Assessment of DFT Exchangeâ€“Correlation Functionals for Evaluating the Multipolar Contributions to the Quadratic Nonlinear Optical Responses of Small Reference Molecules. Journal of Chemical Theory and Computation, 2012, 8, 2044-2052.	2.3	47
460	Electronic structure and spectral properties of the triarylamine-dithienosilole dyes for efficient organic solar cells. Dyes and Pigments, 2012, 92, 531-536.	2.0	53
461	Interstitial water and the formation of low barrier hydrogen bonds: A computational model study. International Journal of Quantum Chemistry, 2012, 112, 1460-1472.	1.0	2
462	Isomerization of dehydrofulvene radicals to the phenyl radical, and application to the growth of polycyclic aromatic hydrocarbons. International Journal of Quantum Chemistry, 2012, 112, 1959-1967.	1.0	1
463	Nï£¿H and Nï£¿Cl homolytic bond dissociation energies and radical stabilization energies: An assessment of theoretical procedures through comparison with benchmarkâ€quality W2w data. International Journal of Quantum Chemistry, 2012, 112, 1862-1878.	1.0	46
464	Spectroscopic properties of monoâ€•and bisâ€azopyrroles. International Journal of Quantum Chemistry, 2012, 112, 2043-2050.	1.0	2
465	Basis set and functional effects on excitedâ€state properties: Three bicyclic chromogens as working examples. International Journal of Quantum Chemistry, 2012, 112, 2135-2141.	1.0	36
466	The electronic spectrum of AgBr₂: Ab initio benchmark calculations on the ²Î_u and ²Î£_u⁺ charge transfer states including spinâ€orbit effects. International Journal of Quantum Chemistry, 2012, 112, 3535-3542.	1.0	2
467	On the Mechanism of the [Cp₂Mo(OH)(OH₂)]⁺-Catalyzed Nitrile Hydration to Amides: A Theoretical Study. Organometallics, 2012, 31, 1618-1626.	1.1	22
468	Computational Studies on Ethylene Addition to Nickel Bis(dithiolene). Journal of Physical Chemistry A, 2012, 116, 476-482.	1.1	37
469	Bonds or not bonds? Pancake bonding in 1,2,3,5-dithiadiazolyl and 1,2,3,5-diselenadiazolyl radical dimers and their derivatives. Physical Chemistry Chemical Physics, 2012, 14, 10713.	1.3	72
470	Structure Properties Relationship of Donorâ€“Acceptor Derivatives of Triphenylamine and 1,8-Naphthalimide. Journal of Physical Chemistry C, 2012, 116, 14811-14819.	1.5	66
471	The Role of Weak Bonding in Determining the Structure of Thiophene Oligomers inside Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 9681-9690.	1.5	26
472	The role of the basis set and the level of quantum mechanical theory in the prediction of the structure and reactivity of cisplatin. Journal of Computational Chemistry, 2012, 33, 2292-2302.	1.5	39

#	Article	IF	Citations
473	Assessment of ab initio MP2 and density functionals for characterizing the potential energy profiles of the S_N2 reactions at N center. Journal of Computational Chemistry, 2012, 33, 1347-1352.	1.5	13
474	Computational Prediction of¹H and¹³C Chemical Shifts: A Useful Tool for Natural Product, Mechanistic, and Synthetic Organic Chemistry. Chemical Reviews, 2012, 112, 1839-1862.	23.0	1,027
475	A Polarizable QM/MM Explicit Solvent Model for Computational Electrochemistry in Water. Journal of Chemical Theory and Computation, 2012, 8, 610-617.	2.3	71
476	Time-dependent density functional theory (TDDFT) modelling of Pechmann dyes: from accurate absorption maximum prediction to virtual dye screening. Organic and Biomolecular Chemistry, 2012, 10, 6682.	1.5	57
477	Geometries and Vibrational Frequencies of Small Radicals: Performance of Coupled Cluster and More Approximate Methods. Journal of Chemical Theory and Computation, 2012, 8, 2165-2179.	2.3	42
478	The entrance complex, transition state, and exit complex for the F + H2O â†' HF + OH reaction. Definitive predictions. Comparison with popular density functional methods. Physical Chemistry Chemical Physics, 2012, 14, 10891.	1.3	63
479	The calculation of active Raman modes of Î±-quartz crystal via density functional theory based on B3LYP Hamiltonian in 6â€“311+G(2d) basis setâ€. Pramana - Journal of Physics, 2012, 78, 803-810.	0.9	5
480	Time-dependent density functional theory benchmarking for the calculations of atomic spectra: efficiency of exc-ETDZ basis set. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	7
481	Generalized gradient exchange functionals based on the gradient-regulated connection: a new member of the TCA family. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	14
482	Can water be a catalyst on the HO2+H2O+O3 reactive cluster?. Chemical Physics, 2012, 399, 17-22.	0.9	19
483	Theoretical investigation of the hydrogen atom transfer in the hydrated Aâ€“T base pair. Chemical Physics, 2012, 394, 9-16.	0.9	17
484	New range-separated hybrids based on the TCA density functional. Chemical Physics Letters, 2012, 519-520, 145-149.	1.2	5
485	The B3LYP and BMK studies of CO adsorption on Pt(1 1 1): An insight through the chemical bonding analysis. Chemical Physics Letters, 2012, 530, 64-70.	1.2	7
486	Structure and spectral properties of truxene dye S5. Optics and Spectroscopy (English Translation of) Tj ETQq1 1 0.784314 rgBT /Ove	0.2	20
487	Structure and spectral properties of triphenylamine dye functionalized with 3,4-propylenedioxythiophene. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2012, 112, 829-835.	0.2	11
488	Hydrogen abstraction reactions of OH radicals with CH₃CH₂CH₂Cl and CH₃CHClCH₃: A mechanistic and kinetic study. Journal of Computational Chemistry, 2012, 33, 66-75.	1.5	7
489	Chemical activation reactions of cyclic alkanes and ethers and tricyclodecane ringâ€opened diradicals with O₂: Thermochemistry, reaction paths, kinetics, and modeling. International Journal of Chemical Kinetics, 2012, 44, 232-256.	1.0	4
490	Density functional theory study of small nickel clusters. Journal of Molecular Modeling, 2012, 18, 783-790.	0.8	36

#	Article	IF	Citations
491	A DFT study on the standard electrode potentials of 2â€substituted imidazoles. International Journal of Quantum Chemistry, 2013, 113, 715-722.	1.0	4
492	Rate constants calculation of hydrogen abstraction reactions CH₃CHBr + HBr and CH₃CBr₂ + HBr. International Journal of Quantum Chemistry, 2013, 113, 997-1002.	1.0	0
493	Density functional and chemical model study of the competition between methyl and hydrogen scission of propane and Î²-scission of the propyl radical. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	8
494	Methodological keys for accurate simulations. Physical Chemistry Chemical Physics, 2013, 15, 11875.	1.3	22
495	Active Thermochemical Tables: Water and Water Dimer. Journal of Physical Chemistry A, 2013, 117, 11940-11953.	1.1	99
496	Dynamic 1H NMR spectroscopic study of hindered internal rotation in selected N,N-dialkyl isonicotinamides: an experimental and DFT analysis. Tetrahedron, 2013, 69, 8147-8154.	1.0	17
497	Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds. Journal of Chemical Theory and Computation, 2013, 9, 3872-3877.	2.3	312
498	Biomimetic Reagents for the Selective Free Radical and Acidâ€"Base Chemistry of Glycans: Application to Glycan Structure Determination by Mass Spectrometry. Journal of the American Chemical Society, 2013, 135, 10684-10692.	6.6	56
499	Barrier Heights in Quantum Monte Carlo with Linear-Scaling Generalized-Valence-Bond Wave Functions. Journal of Chemical Theory and Computation, 2013, 9, 3453-3462.	2.3	15
500	Design of a new axially chiral molecule by conformational fixation: 2,6-dithiaspiro[3.3]heptane 2,6-dioxide and its heavier analogues. Tetrahedron: Asymmetry, 2013, 24, 781-784.	1.8	4
501	Performance of conventional and dispersion-corrected density-functional theory methods for hydrogen bonding interaction energies. Physical Chemistry Chemical Physics, 2013, 15, 12821.	1.3	120
502	Microscopic properties of liquid water from combined ab initio molecular dynamics and energy decomposition studies. Physical Chemistry Chemical Physics, 2013, 15, 15746.	1.3	55
503	Comparison of TD-DFT Methods for the Calculation of Two-Photon Absorption Spectra of Oligophenylvinylenes. Journal of Physical Chemistry C, 2013, 117, 18170-18189.	1.5	68
504	Electrochemistry and time dependent DFT study of a (vinylenedithio)-TTF derivative in different oxidation states. Electrochimica Acta, 2013, 100, 188-196.	2.6	5
505	Blue-Coloured Highly Efficient Dye-Sensitized Solar Cells by Implementing the Diketopyrrolopyrrole Chromophore. Scientific Reports, 2013, 3, 2446.	1.6	143
506	Relating Electron Donor and Carboxylic Acid Anchoring Substitution Effects in Azo Dyes to Dye-Sensitized Solar Cell Performance. ACS Sustainable Chemistry and Engineering, 2013, 1, 1440-1452.	3.2	83
507	Backbone effects on the charge transport in poly-imidazole membranes: a theoretical study. Journal of Materials Chemistry A, 2013, 1, 7751.	5.2	11
508	A computational methodology for accurate predictions of rate constants in solution: Application to the assessment of primary antioxidant activity. Journal of Computational Chemistry, 2013, 34, 2430-2445.	1.5	289

#	Article	IF	Citations
509	A Pd^{II} Complex Bearing a Benzimidazoleâ€Derived Ligand with Potentially â€œMesoionic and Remoteâ€•Character and Its Catalytic Activity. European Journal of Inorganic Chemistry, 2013, 2013, 4654-4661.	1.0	5
510	The study of performance of DFT functional for van der Waals interactions. Computational and Theoretical Chemistry, 2013, 1004, 56-60.	1.1	3
511	Spirooxazine-based multifunctional molecular switches with tunable photochromism and nonlinear optical response. Journal of Materials Chemistry C, 2013, 1, 5779.	2.7	25
512	Avoiding pitfalls of a theoretical approach: the harmonic oscillator measure of aromaticity index from quantum chemistry calculations. Structural Chemistry, 2013, 24, 1171-1184.	1.0	31
513	Performance of Density Functional Theory for Second Row (4d) Transition Metal Thermochemistry. Journal of Chemical Theory and Computation, 2013, 9, 3939-3946.	2.3	74
514	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. , 2013, , 1-57.		1
515	Density functional studies on photophysical properties and chemical reactivities of the triarylboranes: effect of the constraint of planarity. Journal of Molecular Modeling, 2013, 19, 3437-3446.	0.8	11
516	Assessing the quantum mechanical level of theory for prediction of linear and nonlinear optical properties of push-pull organic molecules. Journal of Molecular Modeling, 2013, 19, 2079-2090.	0.8	18
517	Spinâ€componentâ€scaled double hybrids: An extensive search for the best fifthâ€rung functionals blending DFT and perturbation theory. Journal of Computational Chemistry, 2013, 34, 2327-2344.	1.5	292
518	Critical Test of Some Computational Chemistry Methods for Prediction of Gas-Phase Acidities and Basicities. Journal of Chemical Theory and Computation, 2013, 9, 3947-3958.	2.3	38
519	Voltammetry coupled to mass spectrometry in the presence of isotope 18O labeled water for the prediction of oxidative transformation pathways of activated aromatic ethers: Acebutolol. Analytica Chimica Acta, 2013, 762, 39-46.	2.6	17
521	Theoretical studies on the reactions of CHF2CF2OCH3/CH2FCF2OCH3 with OH radicals. Journal of Fluorine Chemistry, 2013, 149, 72-81.	0.9	5
522	Performance of Density Functionals for Activation Energies of Zr-Mediated Reactions. Journal of Chemical Theory and Computation, 2013, 9, 4735-4743.	2.3	62
523	Electronic, Optical, and Computational Studies of a Redox-Active Napthalenediimide-Based Coordination Polymer. Inorganic Chemistry, 2013, 52, 14246-14252.	1.9	37
524	TD-DFT accuracy in determining excited-state structures and fluorescence spectra of firefly emitter. Chemical Research in Chinese Universities, 2013, 29, 982-985.	1.3	4
525	Structure and electronic absorption spectra of isotruxene dyes for dye-sensitized solar cells: Investigation by the DFT, TDDFT, and QTAIM methods. Optics and Spectroscopy (English Translation of) Tj ETQq1 1 0.784314 rgBT /Ov		
527	Molecular hyperpolarizabilities of pushâ€“pull chromophores: A comparison between theoretical and experimental results. Chemical Physics, 2013, 411, 11-16.	0.9	28
528	Assessing the performances of some recently proposed density functionals for the description of organometallic structures. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	12

#	Article	IF	Citations
529	TD-DFT study of the for coumarins. Chemical Physics Letters, 2013, 583, 218-221.	1.2	19
530	Toward extension of the gas-phase basicity scale by novel pyridine containing guanidines. International Journal of Mass Spectrometry, 2013, 354-355, 113-122.	0.7	20
531	An assessment of DFT methods for predicting the thermochemistry of ion-molecule reactions of group 14 elements (Si, Ge, Sn). Journal of Molecular Modeling, 2013, 19, 5439-5444.	0.8	7
532	Benchmark Study of the Performance of Density Functional Theory for Bond Activations with (Ni,Pd)â€Based Transitionâ€Metal Catalysts. ChemistryOpen, 2013, 2, 115-124.	0.9	146
533	Communication: One third: A new recipe for the PBE0 paradigm. Journal of Chemical Physics, 2013, 138, 021104.	1.2	115
534	G3X-K theory: A composite theoretical method for thermochemical kinetics. Chemical Physics Letters, 2013, 558, 109-113.	1.2	46
535	Reaction energetics on longâ€range corrected density functional theory: Dielsâ€“Alder reactions. Journal of Computational Chemistry, 2013, 34, 379-386.	1.5	33
536	Thermochemistry and kinetics of isobutanol oxidation by the OH radical. Fuel, 2013, 106, 431-436.	3.4	10
537	A comparative ab initio study of hydrogen abstraction from n-propyl benzene. Combustion and Flame, 2013, 160, 2642-2653.	2.8	41
538	Assessment of Density Functional Theory for Thermochemical Approaches Based on Bond Separation Reactions. Journal of Physical Chemistry A, 2013, 117, 228-243.	1.1	16
539	Assessing the performance of density functional theory for the dynamic polarizabilities of amino acids: Treatment of correlation and role of exact exchange. International Journal of Quantum Chemistry, 2013, 113, 1803-1811.	1.0	7
540	Assessing the Accuracy of Density Functional and Semiempirical Wave Function Methods for Water Nanoparticles: Comparing Binding and Relative Energies of (H₂O)₁₆ and (H₂O)₁₇ to CCSD(T) Results. Journal of Chemical Theory and Computation, 2013, 9, 995-1006.	2.3	51
541	Neighboring Effect in Fragmentation Pathways of Cage Guanylhydrazones in the Gas Phase. Journal of Physical Chemistry A, 2013, 117, 2242-2252.	1.1	5
542	Torsional barriers of substituted biphenyls calculated using density functional theory: a benchmarking study. Organic and Biomolecular Chemistry, 2013, 11, 2859.	1.5	51
543	Theoretical investigation of hydrogen atom transfer in the hydrated Câ€“G base pair. Molecular Physics, 2013, 111, 201-214.	0.8	11
544	Revisiting the optical signatures of BODIPY with ab initio tools. Chemical Science, 2013, 4, 1950.	3.7	140
545	Design of a new axially chiral molecule by conformational fixation: 2,6-diphospha- and 2,6-diarsaspiro[3.3]heptanes. Tetrahedron: Asymmetry, 2013, 24, 169-171.	1.8	5
546	Are DFT Methods Accurate in Mononuclear Ruthenium-Catalyzed Water Oxidation? An ab Initio Assessment. Journal of Chemical Theory and Computation, 2013, 9, 1872-1879.	2.3	43

#	Article	IF	Citations
547	Halogen Bonds: Benchmarks and Theoretical Analysis. Journal of Chemical Theory and Computation, 2013, 9, 1918-1931.	2.3	435
548	Assessment of density functional methods for thermochemistry of chromium oxo compounds and their application in a study of chromiaâ€“silica system. Chemical Physics Letters, 2013, 561-562, 87-91.	1.2	15
549	A Benchmark Study of H₂ Activation by Au₃ and Ag₃ Clusters. Journal of Physical Chemistry C, 2013, 117, 7487-7496.	1.5	15
550	Shape-Programmed Nanofabrication: Understanding the Reactivity of Dichalcogenide Precursors. ACS Nano, 2013, 7, 3616-3626.	7.3	67
551	Quantum-chemical approach to determining the high potency of clorgyline as an irreversible acetylenic monoamine oxidase inhibitor. Journal of Neural Transmission, 2013, 120, 875-882.	1.4	17
552	The ammonium nitrate and its mechanism of decomposition in the gas phase: a theoretical study and a DFT benchmark. Physical Chemistry Chemical Physics, 2013, 15, 10849.	1.3	43
553	Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. Journal of Chemical Theory and Computation, 2013, 9, 2749-2760.	2.3	243
554	Molecular Engineering of a Fluorene Donor for Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2733-2739.	3.2	154
555	Understanding the Density Functional Dependence of DFT-Calculated Electronic Couplings in Organic Semiconductors. Journal of Physical Chemistry Letters, 2013, 4, 919-924.	2.1	79
556	A simple DFT-based diagnostic for nondynamical correlation. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	114
557	Performance of Density Functional Methods. Some Difficult Cases for Small Systems Containing Cu, Ag, or Au. Journal of Physical Chemistry A, 2013, 117, 2619-2628.	1.1	6
558	Ab Initio Molecular Dynamics Study of the Reaction of U⁺ and U²⁺ with H₂O in the Gas Phase: Direct Classical Trajectory Calculations. Journal of Physical Chemistry A, 2013, 117, 3761-3770.	1.1	10
559	Application of the Generalized Connectivity-Based Hierarchy to Biomonomers: Enthalpies of Formation of Cysteine and Methionine. Journal of Physical Chemistry A, 2013, 117, 4973-4980.	1.1	27
560	Unravelling the Potential for Dithienopyrrole Sensitizers in Dye-Sensitized Solar Cells. Chemistry of Materials, 2013, 25, 2642-2648.	3.2	49
561	Boranil and Related NBO Dyes: Insights From Theory. Journal of Chemical Theory and Computation, 2013, 9, 3127-3135.	2.3	74
562	Acebutolol and alprenolol metabolism predictions: comparative study of electrochemical and cytochrome P450-catalyzed reactions using liquid chromatography coupled to high-resolution mass spectrometry. Analytical and Bioanalytical Chemistry, 2013, 405, 6077-6085.	1.9	26
563	Prediction of Redox Potentials of Adrenaline and Its Supramolecular Complex with Glycine: Theoretical and Experimental Studies. Journal of Physical Chemistry B, 2013, 117, 2081-2087.	1.2	10
564	Which density functional is close to CCSD accuracy to describe geometry and interaction energy of small noncovalent dimers? A benchmark study using Gaussian09. Journal of Computational Chemistry, 2013, 34, 1341-1353.	1.5	108

#	Article	IF	Citations
565	TD-DFT benchmarks: A review. International Journal of Quantum Chemistry, 2013, 113, 2019-2039.	1.0	938
566	Quantum Chemical and Kinetics Study of the Thermal Gas Phase Decomposition of 2-Chloropropene. Journal of Physical Chemistry A, 2013, 117, 10218-10227.	1.1	9
567	Binding in Radical-Solvent Binary Complexes: Benchmark Energies and Performance of Approximate Methods. Journal of Chemical Theory and Computation, 2013, 9, 1568-1579.	2.3	46
568	Effect of Substituents on the Preferred Modes of One-Electron Reductive Cleavage of Nâ€“Cl and Nâ€“Br Bonds. Journal of Physical Chemistry A, 2013, 117, 460-472.	1.1	22
569	Establishing the Accuracy of Broadly Used Density Functionals in Describing Bulk Properties of Transition Metals. Journal of Chemical Theory and Computation, 2013, 9, 1631-1640.	2.3	184
570	First-Principles Molecular Dynamics Simulation of Atmospherically Relevant Anion Solvation in Supercooled Water Droplet. Journal of the American Chemical Society, 2013, 135, 15549-15558.	6.6	32
571	Relaxation of Electronically Excited Hydrogen Peroxide in Liquid Water: Insights from Auger-Electron Emission. Journal of Physical Chemistry C, 2013, 117, 22268-22275.	1.5	13
572	On the Effect of Varying Constraints in the Quantum Mechanics Only Modeling of Enzymatic Reactions: The Case of Acetylene Hydratase. Journal of Physical Chemistry B, 2013, 117, 3954-3961.	1.2	25
573	DFT Study on Homolytic Dissociation Enthalpies of Câ€”I Bonds. Chinese Journal of Chemical Physics, 2013, 26, 541-548.	0.6	10
574	Measuring the internal energies of species emitted from hypervelocity nanoprojectile impacts on surfaces using recalibrated benzylpyridinium probe ions. Journal of Chemical Physics, 2013, 138, 214301.	1.2	17
575	Assessment of theoretical methods for the study of hydrogen abstraction kinetics of global warming gas species during their degradation and byproduct formation (IUPAC Technical Report). Pure and Applied Chemistry, 2013, 85, 1901-1918.	0.9	6
576	Understanding the Electronic Structures and Absorption Properties of Porphyrin Sensitizers YD2 and YD2-o-C8 for Dye-Sensitized Solar Cells. International Journal of Molecular Sciences, 2013, 14, 20171-20188.	1.8	54
577	Understanding the Initial Decomposition Pathways of the nâ€Alkane/Nitroalkane Binary Mixture. Chinese Journal of Chemistry, 2013, 31, 1087-1094.	2.6	12
578	Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals. Physical Review B, 2013, 88, .	1.1	40
579	Valence excitation energies of alkenes, carbonyl compounds, and azabenzenes by time-dependent density functional theory: Linear response of the ground state compared to collinear and noncollinear spin-flip TDDFT with the Tamm-Dancoff approximation. Journal of Chemical Physics, 2013, 138, 134111.	1.2	62
580	Kinetics of Homolytic Substitutions by Hydrogen Atoms at Thiols and Sulfides. ChemPhysChem, 2013, 14, 1703-1722.	1.0	12
582	Assessing the performance of commonly used DFT functionals in studying the chemistry of frustrated Lewis pairs. Journal of Theoretical and Computational Chemistry, 2014, 13, 1350074.	1.8	21
583	Decay Mechanisms of Protonated 4-Quinolone Antibiotics After Electrospray Ionization and Ion Activation. Journal of the American Society for Mass Spectrometry, 2014, 25, 1974-1986.	1.2	23

#	Article	IF	Citations
584	Reaction of Np atom with H2O in the gas phase: reaction mechanisms and ab initio molecular dynamics study. Journal of Molecular Modeling, 2014, 20, 2466.	0.8	3
585	Thermodynamic stability and structural parameters of carbon nanoclusters. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450058.	1.8	4
586	Assessment of theoretical procedures for a diverse set of isomerization reactions involving double-bond migration in conjugated dienes. Chemical Physics, 2014, 441, 166-177.	0.9	49
587	Assessment of density-functionals for describing the Xâ˜ + CH3ONO2 gas-phase reactions with X = F, OH, CH2CN. Physical Chemistry Chemical Physics, 2014, 16, 26769-26778.	1.3	11
588	Insights into the Relationship of Catalytic Activity and Structure: A Comparison Study of Three Carbonic Anhydrase Mimics. International Journal of Chemical Kinetics, 2014, 46, 683-700.	1.0	18
589	Design of Stereoelectronically Promoted Super Lewis Acids and Unprecedented Chemistry of Their Complexes. Chemistry - A European Journal, 2014, 20, 11584-11590.	1.7	12
590	Charge Delocalization in an Organic Mixed Valent Bithiophene Is Greater Than in a Structurally Analogous Biselenophene. Journal of Physical Chemistry A, 2014, 118, 11293-11303.	1.1	20
591	Gasâ€phase water activation by Th atom: Reaction mechanisms and topological analysis. International Journal of Quantum Chemistry, 2014, 114, 760-768.	1.0	14
592	Kinetics of radicalâ€molecule reactions in aqueous solution: A benchmark study of the performance of density functional methods. Journal of Computational Chemistry, 2014, 35, 2019-2026.	1.5	211
593	Coupledâ€cluster reaction barriers of : An application of the coupledâ€cluster//Kohnâ€“Sham density functional theory model chemistry. Journal of Computational Chemistry, 2014, 35, 507-517.	1.5	20
594	Theoretical Chemistry in Belgium. Highlights in Theoretical Chemistry, 2014, , .	0.0	1
595	DNA Lesion Can Facilitate Base Ionization: Vertical Ionization Energies of Aqueous 8-Oxoguanine and its Nucleoside and Nucleotide. Journal of Physical Chemistry B, 2014, 118, 13833-13837.	1.2	13
596	Anthraquinone-Based Intramolecular Charge-Transfer Compounds: Computational Molecular Design, Thermally Activated Delayed Fluorescence, and Highly Efficient Red Electroluminescence. Journal of the American Chemical Society, 2014, 136, 18070-18081.	6.6	822
597	Guanidine and guanidinium cation in the excited stateâ€”theoretical investigation. Journal of Chemical Physics, 2014, 141, 074307.	1.2	5
598	Structure and properties of cerium oxides in bulk and nanoparticulate forms. Journal of Alloys and Compounds, 2014, 584, 199-208.	2.8	79
599	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. Polymer Chemistry, 2014, 5, 524-534.	1.9	12
600	Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120476.	1.6	599
601	Halogen bonds with benzene: An assessment of DFT functionals. Journal of Computational Chemistry, 2014, 35, 386-394.	1.5	73

#	Article	IF	Citations
602	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	37
604	Density Functional Theory in Quantum Chemistry. , 2014, , .		119
605	NIR Emission in Borondifluoride Complexes of 2â€²-Hydroxychalcone Derivatives Containing an Acetonaphthone Ring. Journal of Physical Chemistry C, 2014, 118, 11906-11918.	1.5	24
606	Effects of Heteroatoms on Electronic States of Divanadium-Substituted Î³-Keggin-type Polyoxometalates. Inorganic Chemistry, 2014, 53, 3907-3918.	1.9	13
607	Computational Tests of Quantum Chemical Models for Excited and Ionized States of Molecules with Phosphorus and Sulfur Atoms. Journal of Physical Chemistry A, 2014, 118, 3514-3524.	1.1	5
608	Accurate description of torsion potentials in conjugated polymers using density functionals with reduced self-interaction error. Journal of Chemical Physics, 2014, 140, 054310.	1.2	32
609	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
610	On the Innocence of Bipyridine Ligands: How Well Do DFT Functionals Fare for These Challenging Spin Systems?. Journal of Chemical Theory and Computation, 2014, 10, 220-235.	2.3	34
611	Inorganic chemistry solutions to semiconductor nanocrystal problems. Coordination Chemistry Reviews, 2014, 263-264, 182-196.	9.5	35
612	Conformational Equilibria in Butane-1,4-diol: A Benchmark of a Prototypical System with Strong Intramolecular H-bonds. Journal of Physical Chemistry A, 2014, 118, 293-303.	1.1	53
613	A New-Generation Density Functional. Springer Briefs in Molecular Science, 2014, , .	0.1	20
614	The MC-DFT approach including the SCS-MP2 energies to the new minnesota-type functionals. Journal of Computational Chemistry, 2014, 35, 1560-1567.	1.5	4
615	Computational insight of the mechanism of Algarâ€“Flynnâ€“Oyamada (AFO) reaction. RSC Advances, 2014, 4, 18702.	1.7	17
616	Charting the mechanism and reactivity of zirconium oxalate with hydroxamate ligands using density functional theory: implications in new chelate design. Dalton Transactions, 2014, 43, 9872-9884.	1.6	44
617	Quantum-chemical insights into mixed-valence systems: within and beyond the Robinâ€“Day scheme. Chemical Society Reviews, 2014, 43, 5067-5088.	18.7	168
618	Introducing asymmetry in tetradentate azadipyrromethene chromophores: a systematic study of the impact on electronic and photophysical properties. Physical Chemistry Chemical Physics, 2014, 16, 22207-22221.	1.3	9
619	A RRKM study and a DFT assessment on gas-phase fragmentation of formamideâ€“M2+ (M = Ca, Sr). Physical Chemistry Chemical Physics, 2014, 16, 14813.	1.3	7
620	A theoretical study of the nornicotine-catalyzed Mannich reaction in wet solvents and water. Green Chemistry, 2014, 16, 3999-4008.	4.6	6

#	Article	IF	Citations
621	DFT calculations on kinetic data for some [4+2] reactions in solution. Physical Chemistry Chemical Physics, 2014, 16, 15224.	1.3	38
622	Theoretical insights into the absorption and emission properties of blue luminescent copper(I) complexes based on the pyrazolylâ€pyridine ligands. International Journal of Quantum Chemistry, 2014, 114, 1685-1691.	1.0	4
623	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
624	Accurate prediction of ¹⁹⁵Pt NMR chemical shifts for a series of Pt(<scp>ii</scp>) and Pt(<scp>iv</scp>) antitumor agents by a non-relativistic DFT computational protocol. Dalton Transactions, 2014, 43, 5409-5426.	1.6	36
625	Degradation of methyl salicylate through Cl initiated atmospheric oxidation â€“ a theoretical study. RSC Advances, 2014, 4, 23464.	1.7	26
626	Carbonâ€“Hydrogen Activation of Cycloalkanes by Cyclopentadienylcarbonylrhodiumâ€”A Lifetime Enigma. Journal of the American Chemical Society, 2014, 136, 8614-8625.	6.6	32
627	Prediction of Accurate Thermochemistry of Medium and Large Sized Radicals Using Connectivity-Based Hierarchy (CBH). Journal of Chemical Theory and Computation, 2014, 10, 4342-4350.	2.3	30
628	Electronic descriptors for analytical use of the benzidineâ€based compounds and the mechanism of oxidative coupling of anilines. Journal of Physical Organic Chemistry, 2014, 27, 640-651.	0.9	11
629	Ï‰B97X-V: A 10-parameter, range-separated hybrid, generalized gradient approximation density functional with nonlocal correlation, designed by a survival-of-the-fittest strategy. Physical Chemistry Chemical Physics, 2014, 16, 9904.	1.3	616
630	Performance of Density Functionals for Activation Energies of Re-Catalyzed Organic Reactions. Journal of Chemical Theory and Computation, 2014, 10, 579-588.	2.3	47
631	A Theoretical Study On Rh(I) Catalyzed Enantioselective Conjugate Addition Reactions of Fluoroalkylated Olefins. Organometallics, 2014, 33, 5111-5119.	1.1	8
632	A theoretical study on the mechanism and dynamics of reactions (CF₃)₂CHOCH₂F/(CF₃)₂CHOCHF₂with OH radical. Molecular Physics, 2014, 112, 2987-2996.		1
633	Reactions of Benzene and 3-Methylpyrrole with the â€¢OH and â€¢OOH Radicals: An Assessment of Contemporary Density Functional Theory Methods. Journal of Physical Chemistry A, 2014, 118, 2667-2682.	1.1	7
634	Experimental and DFT/Time-Dependent DFT Studies on Neutral and One-Electron-Reduced Quinoxaline and Pyrazine Precursors and Their Mononuclear (PdII, PtII) Derivatives. European Journal of Inorganic Chemistry, 2014, 2014, 3572-3581.	1.0	4
635	Effect of Protonation State and Interposed Connector Groups on Bond Dissociation Enthalpies of Alcohols and Related Systems. Journal of Physical Chemistry A, 2014, 118, 2810-2819.	1.1	30
636	Performance of Density Functional Theory Procedures for the Calculation of Proton-Exchange Barriers: Unusual Behavior of M06-Type Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3777-3783.	2.3	44
637	Reactions of an Isolable Dialkylsilylene with Carbon Dioxide and Related Heterocumulenes. Organometallics, 2014, 33, 5434-5439.	1.1	57
638	Chlorination of N-Methylacetamide and Amide-Containing Pharmaceuticals. Quantum-Chemical Study of the Reaction Mechanism. Journal of Physical Chemistry A, 2014, 118, 2367-2376.	1.1	20

#	Article	IF	Citations
639	Theoretical study on dynamics of the gas phase reactions of CF 3 CF 2 CH 2 OCHF 2 with OH radicals. Journal of Fluorine Chemistry, 2014, 168, 25-33.	0.9	2
640	Benchmarking of Density Functionals for the Accurate Description of Thiolâ€“Disulfide Exchange. Journal of Chemical Theory and Computation, 2014, 10, 4842-4856.	2.3	33
641	Assessing the Performance of CASPT2 and DFT Methods for the Description of Long, Multicenter Bonding in Dimers between Radical Ions. Journal of Chemical Theory and Computation, 2014, 10, 650-658.	2.3	29
642	Performance of recent density functionals to discriminate between olefin and nitrogen binding to palladium. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	7
643	Comparative study of Gaussian basis sets for calculation of core electron binding energies in first-row hydrides and glycine. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	12
644	Photoinduced excited state intramolecular proton transfer of 2-(2â€²-hydroxyphenyl)phenanthro[9,10-d]oxazole: A comprehensive theoretical study. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 294, 14-19.	2.0	3
645	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. Organic and Biomolecular Chemistry, 2014, 12, 7270-7278.	1.5	11
646	Performance of density functionals for computation of core electron binding energies in first-row hydrides and glycine. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	11
647	Stereoselective propagation in free radical polymerization of acrylamides: A DFT study. Journal of Molecular Graphics and Modelling, 2014, 49, 55-67.	1.3	8
648	Microkinetic modeling of CO2 hydrolysis over Zn-(1,4,7,10-tetraazacyclododecane) catalyst based on first principles: Revelation of rate-determining step. Journal of Catalysis, 2014, 317, 176-184.	3.1	19
649	Experimental and theoretical evidence suggests carbamate intermediates play a key role in CO2 sequestration catalysed by sterically hindered amines. Structural Chemistry, 2014, 25, 1535-1546.	1.0	13
651	Photophysical and Electrochemical Properties of Thienylnaphthalimide Dyes with Excellent Photostability. Journal of Physical Chemistry A, 2014, 118, 5178-5188.	1.1	13
652	Theoretical kinetic study of the unimolecular decomposition of 2-bromopropene. Chemical Physics Letters, 2014, 608, 386-392.	1.2	4
653	Quantum mechanistic insights on aryl propargyl ether Claisen rearrangement. Organic and Biomolecular Chemistry, 2014, 12, 4163-4171.	1.5	14
654	Predicting pKa in Implicit Solvents: Current Status and Future Directions. Australian Journal of Chemistry, 2014, 67, 1441.	0.5	91
655	Modeling Spin-Forbidden Monomer Self-Initiation Reactions in Spontaneous Free-Radical Polymerization of Acrylates and Methacrylates. Journal of Physical Chemistry A, 2014, 118, 9310-9318.	1.1	34
656	The role of terminal groups in electronic structures and related properties: The case of pushâ€“pull porphyrin dye sensitizers for solar cells. Computational and Theoretical Chemistry, 2014, 1039, 62-70.	1.1	12
657	The mechanism and dynamic studies for the reactions of OH radical with CH3â^'nFnOCF2CHFCl (n=0, 1,) Tj ETQq1 1 0.784314 rgBT /Ov	0.9	2

#	Article	IF	Citations
658	Quantum mechanical investigations on the role of neutral and negatively charged enamine intermediates in organocatalyzed reactions. Chemical Physics, 2014, 434, 30-36.	0.9	9
659	Environmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test cases. Computational and Theoretical Chemistry, 2014, 1037, 35-48.	1.1	21
660	The theoretical assessment and prediction of CBr bond dissociation enthalpies. Computational and Theoretical Chemistry, 2014, 1027, 116-124.	1.1	14
661	Shock wave and modeling study of the thermal decomposition reactions of pentafluoroethane and 2-H-heptafluoropropane. Physical Chemistry Chemical Physics, 2014, 16, 9797-9807.	1.3	11
662	Mixedâ€Valence Ruthenium Complexes Rotating through a Conformational Robinâ€“Day Continuum. Chemistry - A European Journal, 2014, 20, 6895-6908.	1.7	76
663	Probing the relationship between spin contamination and first hyperpolarizability: Openâ€shell MÃ¶bius anion. International Journal of Quantum Chemistry, 2014, 114, 720-724.	1.0	1
664	Absolute configuration of 1,5-diazepin-2-ones: A critical test case for density functional theory. Computational and Theoretical Chemistry, 2014, 1044, 15-23.	1.1	4
665	Investigation of the reactions of U, U⁺and U²⁺with ammonia: mechanisms and topological analysis. RSC Advances, 2014, 4, 29806.	1.7	20
666	Reprint of â€œEnvironmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test casesâ€• Computational and Theoretical Chemistry, 2014, 1040-1041, 144-157.	1.1	1
667	Double-hybrid density-functional theory with meta-generalized-gradient approximations. Journal of Chemical Physics, 2014, 140, 084107.	1.2	35
668	SN2 Reaction of IOâ¯ + CH3Cl: An Ab Initio and DFT Benchmark Study. Bulletin of the Chemical Society of Japan, 2015, 88, 110-116.	2.0	4
669	Following the molecular motion of near-resonant excited CO on Pt(111): A simulated x-ray photoelectron diffraction study based on molecular dynamics calculations. Structural Dynamics, 2015, 2, 035102.	0.9	6
670	A Theoretical Study of Ene Reactions in Solution: A Solutionâ€Phase Translational Entropy Model. ChemPhysChem, 2015, 16, 3711-3718.	1.0	20
671	A Computational Comparison of Oxygen Atom Transfer Catalyzed by Dimethyl SulfÂoxide Reductase with Mo and W. European Journal of Inorganic Chemistry, 2015, 2015, 3580-3589.	1.0	23
672	Unexpected benzimidazole ring formation from a quinoneimide species in the presence of ammonium acetate as supporting electrolyte used in the coupling of electrochemistry with mass spectrometry. Rapid Communications in Mass Spectrometry, 2015, 29, 456-460.	0.7	4
673	A Quantum Mechanical Study on the Propagation Kinetics ofN-methylacrylamide: Comparison WithN,N-Dimethylacrylamide in Free Radical Polymerization. Macromolecular Theory and Simulations, 2015, 24, 218-231.	0.6	2
674	Critical evaluation of the potential energy surface of the CH3 + HO2reaction system. Journal of Chemical Physics, 2015, 142, 054308.	1.2	11
675	Computational studies on hypervalent iodonium(III) compounds as activated precursors for 18F radiofluorination of electron-rich arenes. Computational and Theoretical Chemistry, 2015, 1066, 34-46.	1.1	14

#	Article	IF	Citations
676	Computational Molecular Electronic Spectroscopy with TD-DFT. Topics in Current Chemistry, 2015, 368, 347-375.	4.0	29
677	Theoretical investigation of HNgNH3+ ions (Ng = He, Ne, Ar, Kr, and Xe). Journal of Chemical Physics, 2015, 142, 144301.	1.2	6
678	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 C1â€“C5 oxygenates. Molecular Physics, 2015, 113, 1630-1635.	0.8	8
679	Nonâ€enzymatic Ribonucleotide Reduction in the Prebiotic Context. Chemistry - A European Journal, 2015, 21, 6132-6143.	1.7	7
680	Quantum-chemical investigation of the structure and electronic absorption spectra of symmetric triphenylamine oligomers conjugated to vinylene, imine, azine, and ethynylene groups. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2015, 118, 703-710.	0.2	2
681	Atmospheric reactivity of HCî€,CCH2OH (2-propyn-1-ol) toward OH radicals: experimental determination and theoretical comparison with its alkyne analogue. RSC Advances, 2015, 5, 106668-106679.	1.7	0
682	Assessing density functionals for the prediction of thermochemistry of Tiâ€“Oâ€“Cl species. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550055.	1.8	2
683	Toward understanding the activity of cobalt carbonic anhydrase: A comparative study of zinc- and cobalt-cyclen. Applied Catalysis A: General, 2015, 492, 151-159.	2.2	11
684	Electrochemical oxidation stability of anions for modern battery electrolytes: a CBS and DFT study. Physical Chemistry Chemical Physics, 2015, 17, 3697-3703.	1.3	31
685	Experimental and Computational Insights into Carbon Dioxide Fixation by RZnOH Species. Chemistry - A European Journal, 2015, 21, 5496-5503.	1.7	10
686	Carotenoids and Light-Harvesting: From DFT/MRCI to the Tammâ€“Dancoff Approximation. Journal of Chemical Theory and Computation, 2015, 11, 655-666.	2.3	44
687	Functional tuning of organic dyes containing 2,7-carbazole and other electron-rich segments in the conjugation pathway. RSC Advances, 2015, 5, 17953-17966.	1.7	20
688	Density Functional Theory and Hydrogen Bonds: Are We There Yet?. ChemPhysChem, 2015, 16, 978-985.	1.0	129
689	Electron-Deficient Heteroarenium Salts: An Organocatalytic Tool for Activation of Hydrogen Peroxide in Oxidations. Journal of Organic Chemistry, 2015, 80, 2676-2699.	1.7	43
690	Computational Mechanistic Studies on Reactions of Transition Metal Complexes with Noninnocent Pincer Ligands: Aromatizationâ€“Dearomatization or Not. ACS Catalysis, 2015, 5, 1895-1913.	5.5	75
691	Accurate reaction barrier heights of pericyclic reactions: Surprisingly large deviations for the <scp>CBSâ€QB3</scp> composite method and their consequences in <scp>DFT</scp> benchmark studies. Journal of Computational Chemistry, 2015, 36, 622-632.	1.5	124
692	Computational prediction for emission energy of iridium (III) complexes based on TDDFT calculations using exchange-correlation functionals containing various HF exchange percentages. Journal of Molecular Modeling, 2015, 21, 22.	0.8	7
693	A theoretical study on Câ€“H bond dissociation enthalpies of oxygen-containing fused heterocyclic compounds. Research on Chemical Intermediates, 2015, 41, 7207-7225.	1.3	1

#	Article	IF	Citations
694	Comparative Assessment of DFT Performances in Ru- and Rh-Promoted Ïƒ-Bond Activations. Journal of Chemical Theory and Computation, 2015, 11, 1428-1438.	2.3	45
695	A comparison of the Câ€'H bond dissociation enthalpies of sulfur-containing fused heterocyclic compounds to the Câ€'H bond dissociation enthalpies in other heterocycles. Journal of Sulfur Chemistry, 2015, 36, 155-169.	1.0	7
696	Symmetry-Breaking in Cationic Polymethine Dyes: Part 2. Shape of Electronic Absorption Bands Explained by the Thermal Fluctuations of the Solvent Reaction Field. Journal of Physical Chemistry A, 2015, 119, 6807-6815.	1.1	39
697	Reaction barrier heights for cycloreversion of heterocyclic rings: An Achillesâ€™ heel for DFT and standard ab initio procedures. Chemical Physics, 2015, 458, 1-8.	0.9	68
698	A theoretical investigation of the atmospherically important reaction between chlorine atoms and formic acid: determination of the reaction mechanism and calculation of the rate coefficient at different temperatures. Molecular Physics, 2015, 113, 1511-1533.	0.8	8
699	JP-10 combustion studied with shock tube experiments and modeled with automatic reaction mechanism generation. Combustion and Flame, 2015, 162, 3115-3129.	2.8	80
700	Choosing a density functional for static molecular polarizabilities. Chemical Physics Letters, 2015, 635, 257-261.	1.2	39
701	Theoretical studies on a carbonaceous molecular bearing: association thermodynamics and dual-mode rolling dynamics. Chemical Science, 2015, 6, 2746-2753.	3.7	56
702	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
703	Kinetics and Products of Vinyl + 1,3-Butadiene, a Potential Route to Benzene. Journal of Physical Chemistry A, 2015, 119, 7325-7338.	1.1	20
704	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. Highlights in Theoretical Chemistry, 2015, , 233-246.	0.0	1
705	Group Additive Kinetics for Hydrogen Transfer Between Oxygenates. Journal of Physical Chemistry A, 2015, 119, 6961-6980.	1.1	16
706	The electronic structure engineering of organic dye sensitizers for solar cells: The case of JK derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 855-866.	2.0	6
707	Quantum mechanical study of the kinetics, mechanisms and thermodynamics of the gas-phase decomposition of Pb[(iPr)2PSSe]2 single-source precursor. Journal of Organometallic Chemistry, 2015, 787, 33-43.	0.8	3
708	H and D Attachment to Naphthalene: Spectra and Thermochemistry of Cold Gas-Phase 1-C₁₀H₉ and 1-C₁₀H₈D Radicals and Cations. Journal of Physical Chemistry A, 2015, 119, 3225-3232.	1.1	10
709	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
710	Assessing accuracy of exchangeâ€“correlation functionals for singletâ€“triplet excitations. Computational and Theoretical Chemistry, 2015, 1060, 52-57.	1.1	2
711	Homolytic Câ€“O Cleavage in Phosphates and Sulfonates. Journal of Physical Chemistry A, 2015, 119, 3488-3499.	1.1	7

#	Article	IF	Citations
712	Mapping the genome of meta-generalized gradient approximation density functionals: The search for B97M-V. Journal of Chemical Physics, 2015, 142, 074111.	1.2	305
713	Regarding the use and misuse of retinal protonated Schiff base photochemistry as a test case for time-dependent density-functional theory. Journal of Chemical Physics, 2015, 142, 144104.	1.2	15
714	A kinetic and thermochemical database for organic sulfur and oxygen compounds. Physical Chemistry Chemical Physics, 2015, 17, 13625-13639.	1.3	16
715	The electronic, optical and magnetic consequences of delocalization in multifunctional donorâ€“acceptor organic polymers. Physical Chemistry Chemical Physics, 2015, 17, 11252-11259.	1.3	17
716	Modeling Photoionization of Aqueous DNA and Its Components. Accounts of Chemical Research, 2015, 48, 1209-1217.	7.6	67
717	Beyond Energies: Geometries of Nonbonded Molecular Complexes as Metrics for Assessing Electronic Structure Approaches. Journal of Chemical Theory and Computation, 2015, 11, 1481-1492.	2.3	90
718	Ultraviolet photochemical reaction of [Fe(III)(C2O4)3]3â^' in aqueous solutions studied by femtosecond time-resolved X-ray absorption spectroscopy using an X-ray free electron laser. Structural Dynamics, 2015, 2, 034901.	0.9	52
719	Elucidation of hydrogen-release mechanism from methylamine in the presence of borane, alane, diborane, dialane, and boraneâ€“alane. Molecular Physics, 2015, 113, 79-88.	0.8	2
720	Computations Reveal a Rich Mechanistic Variation of Demethylation of N-Methylated DNA/RNA Nucleotides by FTO. ACS Catalysis, 2015, 5, 7077-7090.	5.5	56
721	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. Journal of Chemical Physics, 2015, 143, 054107.	1.2	605
722	Investigation of the mechanism of electron capture and electron transfer dissociation of peptides with a covalently attached free radical hydrogen atom scavenger. International Journal of Mass Spectrometry, 2015, 390, 49-55.	0.7	11
723	Assessment of DFT Methods for Computing Activation Energies of Mo/W-Mediated Reactions. Journal of Chemical Theory and Computation, 2015, 11, 4601-4614.	2.3	52
724	Photochromic Diarylethenes with Heterocyclic Aromatic Rings: Correlation between Thermal Bistability and Geometrical Characters of Transition States. Journal of Physical Chemistry A, 2015, 119, 9140-9147.	1.1	14
725	Theoretical study on homolytic C(sp2)â€“O cleavage in ethers and phenols. New Journal of Chemistry, 2015, 39, 6935-6943.	1.4	7
726	Critical test of some computational methods for prediction of NMR 1H and 13C chemical shifts. Journal of Molecular Modeling, 2015, 21, 244.	0.8	30
727	Quantum chemical study of small BnCm cluster structures and their physical properties. European Physical Journal D, 2015, 69, 1.	0.6	24
728	Reactivity of Dimeric Tetrazirconium(IV) Wellsâ€“Dawson Polyoxometalate toward Dipeptide Hydrolysis Studied by a Combined Experimental and Density Functional Theory Approach. Inorganic Chemistry, 2015, 54, 11477-11492.	1.9	32
729	Mechanisms and energetics of free radical initiated disulfide bond cleavage in model peptides and insulin by mass spectrometry. Chemical Science, 2015, 6, 4550-4560.	3.7	30

#	Article	IF	Citations
730	An assessment of theoretical procedures forÏ€-conjugation stabilisation energies in enones. Molecular Physics, 2015, 113, 1284-1296.	0.8	19
731	Excited States of Ladder-Type Ï€-Conjugated Dyes with a Joint SOS-CIS(D) and PCM-TD-DFT Approach. Journal of Physical Chemistry A, 2015, 119, 5417-5425.	1.1	13
732	Influence of the Density Functional and Basis Set on the Relative Stabilities of Oxygenated Isomers of Diiron Models for the Active Site of [FeFe]-Hydrogenase. Journal of Chemical Theory and Computation, 2015, 11, 205-214.	2.3	13
733	Investigating the nature of intermolecular and intramolecular bonds in noble gas containing molecules. International Journal of Quantum Chemistry, 2015, 115, 165-171.	1.0	1
734	Theoretical investigation on a series of novel S,S-dioxide diarylethenes with abnormal photochromic properties and design of new dyads. New Journal of Chemistry, 2015, 39, 1634-1642.	1.4	12
735	Tuning optical and electronic properties of poly(4,4'-triphenylamine vinylene)s by post-modification reactions. Dyes and Pigments, 2015, 113, 227-238.	2.0	10
736	Frequency and Zero-Point Vibrational Energy Scale Factors for Double-Hybrid Density Functionals (and Other Selected Methods): Can Anharmonic Force Fields Be Avoided?. Journal of Physical Chemistry A, 2015, 119, 1701-1714.	1.1	441
737	DFT and TD-DFT Assessment of the Structural and Optoelectronic Properties of an Organicâ€“Ag₁₄ Nanocluster. Journal of Physical Chemistry A, 2015, 119, 5088-5098.	1.1	31
739	New Vistas on the Anionic Polymerization of Styrene in Non-Polar Solvents by Means of Density Functional Theory. Polymers, 2016, 8, 371.	2.0	7
740	Performance of the OP correlation functional in relation to its formulation: Influence of the exchange component and the effect of incorporating same-spin correlations. Journal of Computational Chemistry, 2016, 37, 1306-1312.	1.5	5
741	Synthesis, Structure, and Optical Studies of Donorâ€“Acceptorâ€Type Nearâ€Infrared (NIR) Azaâ€“Boronâ€Dipyrromethene (BODIPY) Dyes. Chemistry - an Asian Journal, 2016, 11, 1572-1587.	1.7	41
742	Excited-State Dipole and Quadrupole Moments: TD-DFT versus CC2. Journal of Chemical Theory and Computation, 2016, 12, 3993-4003.	2.3	41
744	The Intersection of NO and H₂S: Persulfides Generate NO from Nitrite through Polysulfide Formation. Inorganic Chemistry, 2016, 55, 12618-12625.	1.9	43
745	Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections. Journal of Chemical Physics, 2016, 145, 204101.	1.2	26
746	Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. Journal of Chemical Physics, 2016, 144, 074106.	1.2	117
747	Ï‰B97M-V: A combinatorially optimized, range-separated hybrid, meta-GGA density functional with VV10 nonlocal correlation. Journal of Chemical Physics, 2016, 144, 214110.	1.2	595
748	Exciton Splitting of Adsorbed and Free 4-Nitroazobenzene Dimers: A Quantum Chemical Study. Journal of Physical Chemistry A, 2016, 120, 3055-3070.	1.1	16
749	Role of (H₂O)_n (n = 2â€“3) Clusters on the HO₂ + O₃ Reaction: A Theoretical Study. Journal of Physical Chemistry B, 2016, 120, 1560-1568.	1.2	26

#	Article	IF	Citations
750	Theoretical study on the mechanism of thieno[3,2â€b]benzofuran bromination: the importance of Lewis and nonâ€Lewis type NBOs interactions along the reaction path. Journal of Physical Organic Chemistry, 2016, 29, 21-28.	0.9	4
751	A dataset of highly accurate homolytic Nï£¿Br bond dissociation energies obtained by Means of W2 theory. International Journal of Quantum Chemistry, 2016, 116, 52-60.	1.0	28
752	The optical signature of 2,6-bis((E)-2-(benzoxazol-2-yl)vinyl)naphthalene (BBVN) laser dye: a TDDFT study. New Journal of Chemistry, 2016, 40, 4911-4921.	1.4	1
753	Hydrogen transfer between dimethyl ether and the methoxy radical: Understanding and kinetic modeling with anharmonic torsions. Computational and Theoretical Chemistry, 2016, 1089, 43-53.	1.1	6
754	DFT Methods to Study the Reaction Mechanism of Iridiumâ€Catalyzed Hydrogenation of Olefins: Which Functional Should be Chosen?. ChemPhysChem, 2016, 17, 119-127.	1.0	14
755	Density functional theory study of the mechanism of a dipeptide-catalyzed intermolecular aldol reactionâ€"the effects of steric repulsion interactions on stereoselectivity. RSC Advances, 2016, 6, 19742-19750.	1.7	2
756	Thermal Decomposition of 3-Bromopropene. A Theoretical Kinetic Investigation. Journal of Physical Chemistry A, 2016, 120, 2285-2294.	1.1	6
757	Density functional investigation of CO and NO adsorption on TM-decorated C60 fullerene. Applied Surface Science, 2016, 383, 353-366.	3.1	35
758	Highly Directional 1D Supramolecular Assembly of New Diketopyrrolopyrrole-Based Gel for Organic Solar Cell Applications. Langmuir, 2016, 32, 4346-4351.	1.6	48
759	Choosing an appropriate model chemistry in a big data context: Application to dative bonding. Computational and Theoretical Chemistry, 2016, 1085, 46-55.	1.1	2
760	Dispersion-Corrected Mean-Field Electronic Structure Methods. Chemical Reviews, 2016, 116, 5105-5154.	23.0	1,032
761	Electrochemical and Spectroscopic Properties of Boron Dipyrromethaneâ€"Thiopheneâ€"Triphenylamine-Based Dyes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2016, 120, 9068-9080.	1.5	36
762	Orbital theory for diastereoselectivity in electrophilic addition. Tetrahedron Letters, 2016, 57, 2029-2033.	0.7	2
763	The effects of exact exchange of density functionals on the evaluation of second hyperpolarizabilities of streptocyanines using sum-over-states method. Computational and Theoretical Chemistry, 2016, 1085, 40-45.	1.1	6
764	Comprehensive Energetic Scale for Quantitatively Estimating the Fluorinating Potential of Nâ€"F Reagents in Electrophilic Fluorinations. Journal of Organic Chemistry, 2016, 81, 4280-4289.	1.7	50
765	MN15: A Kohnâ€"Sham global-hybrid exchangeâ€"correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. Chemical Science, 2016, 7, 5032-5051.	3.7	858
766	A detailed combined experimental and theoretical study on dimethyl ether/propane blended oxidation. Combustion and Flame, 2016, 168, 310-330.	2.8	85
767	Insights into the reaction mechanism of 3-O-sulfotransferase through QM/MM calculations. Physical Chemistry Chemical Physics, 2016, 18, 11488-11496.	1.3	11

#	Article	IF	Citations
768	Theoretical investigation of the singletâ€“triplet splittings for carbazole-based thermally activated delayed fluorescence emitters. Physical Chemistry Chemical Physics, 2016, 18, 26623-26629.	1.3	47
769	Reactivity of electrophilic chlorine atoms due to Ï*f*-holes: a mechanistic assessment of the chemical reduction of a trichloromethyl group by sulfur nucleophiles. Physical Chemistry Chemical Physics, 2016, 18, 27300-27307.	1.3	9
770	Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. Chemical Communications, 2016, 52, 13840-13860.	2.2	18
771	Mechanism of reaction CH3COCl with HNO: A theoretical study. Computational and Theoretical Chemistry, 2016, 1096, 40-44.	1.1	1
772	Density Functional Theory. Encyclopedia of Earth Sciences Series, 2016, , 1-7.	0.1	2
773	Benchmarking the DFT methodology for assessing antioxidant-related properties: quercetin and edaravone as case studies. Journal of Molecular Modeling, 2016, 22, 250.	0.8	24
774	Coupled molecular design diagrams to guide safer chemical design with reduced likelihood of perturbing the NRF2-ARE antioxidant pathway and inducing cytotoxicity. Green Chemistry, 2016, 18, 6387-6394.	4.6	7
775	Understanding and modeling the hydrogen-abstraction from dimethyl ether by the methyl radical with torsional anharmonicity. Computational and Theoretical Chemistry, 2016, 1096, 7-16.	1.1	3
776	Theoretical investigations of the small molecular acceptor materials based on oligothiophene â€“ naphthalene diimide in organic solar cells. RSC Advances, 2016, 6, 102159-102171.	1.7	9
777	Origin of the Different Reactivity of the Triatomic Anions HMoN^{â€“} and ZrNH^{â€“} toward Alkane: Compositions of the Active Orbitals. Journal of Physical Chemistry A, 2016, 120, 7786-7791.	1.1	4
778	The 1,2-hydrogen shift reaction for monohalogenophosphanes PH₂X and HPX (XÂ= F, Cl). Molecular Physics, 2016, 114, 2999-3014.	0.8	3
779	The Effect of Alcohol and Carbonyl Functional Groups on the Competition between Unimolecular Decomposition and Isomerization in C₄ and C₅ Alkoxy Radicals. International Journal of Chemical Kinetics, 2016, 48, 544-555.	1.0	1
780	Benchmark Calculations of Energetic Properties of Groups 4 and 6 Transition Metal Oxide Nanoclusters Including Comparison to Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 3689-3710.	2.3	32
781	A comparative examination of density functional performance against the ISOL24/11 isomerization energy benchmark. Computational and Theoretical Chemistry, 2016, 1090, 147-152.	1.1	23
782	An Organic Dyad Composed of Diathiafulvaleneâ€Functionalized Diketopyrrolopyrroleâ€“Fullerene for Singleâ€Component Highâ€Efficiency Organic Solar Cells. Angewandte Chemie - International Edition, 2016, 55, 12334-12337.	7.2	56
783	An Organic Dyad Composed of Diathiafulvaleneâ€Functionalized Diketopyrrolopyrroleâ€“Fullerene for Singleâ€Component Highâ€Efficiency Organic Solar Cells. Angewandte Chemie, 2016, 128, 12522-12525.	1.6	9
784	Efficient Roomâ€Temperature Methane Activation by the Closedâ€Shell, Metalâ€Free Cluster [OSiOH]⁺: A Novel Mechanistic Variant. Chemistry - A European Journal, 2016, 22, 14257-14263.	1.7	13
785	Kineticâ€energyâ€density dependent semilocal exchangeâ€correlation functionals. International Journal of Quantum Chemistry, 2016, 116, 1641-1694.	1.0	78

#	Article	IF	Citations
786	Molecular Insight from DFT Computations and Kinetic Measurements into the Steric Factors Influencing Peptide Bond Hydrolysis Catalyzed by a Dimeric Zr(IV)-Substituted Keggin Type Polyoxometalate. Inorganic Chemistry, 2016, 55, 9316-9328.	1.9	30
787	Insights on the Auxochromic Properties of the Guanidinium Group. Journal of Physical Chemistry A, 2016, 120, 7088-7100.	1.1	15
788	Structural and Electronic Property Study of (ZnO)_n, n â‰ 168: Transition from Zinc Oxide Molecular Clusters to Ultrasmall Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 20400-20418.	1.5	53
789	Modelling fluorescence lifetimes with TD-DFT: a case study with syn-bimanes. RSC Advances, 2016, 6, 87237-87245.	1.7	13
790	A unified set of experimental organometallic data used to evaluate modern theoretical methods. Dalton Transactions, 2016, 45, 13766-13778.	1.6	24
791	Probabilistic diagram for designing chemicals with reduced potency to incur cytotoxicity. Green Chemistry, 2016, 18, 4461-4467.	4.6	11
792	[Al₂O₄]^{â^'}, a Benchmark Gas-Phase Class II Mixed-Valence Radical Anion for the Evaluation of Quantum-Chemical Methods. Journal of Chemical Theory and Computation, 2016, 12, 3796-3806.	2.3	20
793	The <scp>XYG3</scp> type of doubly hybrid density functionals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 721-747.	6.2	52
794	Revisiting alternative pathways in the Fischerâ€“Tropsch process: Accurate density functional theory calculations on â€œmagicâ€•Ru₁₂ clusters. International Journal of Quantum Chemistry, 2016, 116, 1451-1458.	1.0	2
795	Performance of Hybrid DFT Compared to MP2 Methods in Calculating Nonlinear Optical Properties of Divinylpyrene Derivative Molecules. Journal of Physical Chemistry A, 2016, 120, 8843-8852.	1.1	43
796	Restricted-Open-Shell G4(MP2)-Type Procedures. Journal of Physical Chemistry A, 2016, 120, 9299-9304.	1.1	19
797	Substrate Sulfoxidation by an Iron(IV)-Oxo Complex: Benchmarking Computationally Calculated Barrier Heights to Experiment. Journal of Physical Chemistry A, 2016, 120, 9805-9814.	1.1	80
798	Analysis of the electronic, IR, and 1H NMR spectra of conjugated oligomers based on 4,4'-triphenylamine vinylene. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2016, 121, 348-356.	0.2	4
799	Cooperative Effects in Clusters and Oligonuclear Complexes of Transition Metals in Isolation. Structure and Bonding, 2016, , 1-40.	1.0	5
800	Assessment of quantum chemical methods for the calculation of homolytic Nâ€“F bond dissociation energies. Chemical Data Collections, 2016, 5-6, 28-35.	1.1	5
801	Accurate description of hybridized local and charge-transfer excited-state in donorâ€“acceptor molecules using density functional theory. RSC Advances, 2016, 6, 108404-108410.	1.7	23
802	A DFT kinetic study on 1,3-dipolar cycloaddition reactions in solution. Physical Chemistry Chemical Physics, 2016, 18, 30815-30823.	1.3	32
803	Activation of Methane and Ethane as Mediated by the Triatomic Anion HNbN^{â^'}: Electronic Structure Similarity with a Pt Atom. Angewandte Chemie, 2016, 128, 5031-5035.	1.6	11

#	Article	IF	Citations
804	Activation of Methane and Ethane as Mediated by the Triatomic Anion HNbN^{â˜}: Electronic Structure Similarity with a Pt Atom. Angewandte Chemie - International Edition, 2016, 55, 4947-4951.	7.2	36
805	Computation Sheds Insight into Iron Porphyrin Carbenesâ€™ Electronic Structure, Formation, and Nâ€“H Insertion Reactivity. Journal of the American Chemical Society, 2016, 138, 9597-9610.	6.6	99
806	Photochemistry of Nitrophenol Molecules and Clusters: Intra- vs Intermolecular Hydrogen Bond Dynamics. Journal of Physical Chemistry A, 2016, 120, 4139-4146.	1.1	13
807	Theoretical kinetic study of the reaction of SF5 radical with F2, Cl2 and SF5. Computational and Theoretical Chemistry, 2016, 1090, 41-46.	1.1	5
808	Theoretical investigation on correlation between steric effects and selectivity in gasâ€“solid chlorination of polyvinyl chloride. Chemical Engineering Science, 2016, 151, 64-78.	1.9	6
809	Theoretical study on the mechanism of chloroacetyl chloride decomposition. Computational and Theoretical Chemistry, 2016, 1086, 52-57.	1.1	1
810	Bis(diphenylamino)naphthalene host materials: careful selection of the substitution pattern for the design of fully solution-processed triple-layered electroluminescent devices. RSC Advances, 2016, 6, 60565-60577.	1.7	7
811	Spirooxazine-Fulgide Biphotochromic Molecular Switches with Nonlinear Optical Responses across Four States. Journal of Physical Chemistry C, 2016, 120, 14840-14853.	1.5	37
812	Can nitro groups really anchor onto TiO₂? Case study of dye-to-TiO₂adsorption using azo dyes with NO₂substituents. Physical Chemistry Chemical Physics, 2016, 18, 19062-19069.	1.3	28
813	Preparation of an ion with the highest calculated proton affinity: ortho-diethynylbenzene dianion. Chemical Science, 2016, 7, 6245-6250.	3.7	19
814	Beyond the Halogen Bond: Examining the Limits of Extended Polybromide Networks through Quantumâ€Chemical Investigations. Chemistry - an Asian Journal, 2016, 11, 682-686.	1.7	9
815	Gradient-regulated connection-based correction for the PBE exchange: the PBEtrans model. Molecular Physics, 2016, 114, 1059-1065.	0.8	3
816	Electronic structure and spectral properties of aurones as visible range fluorescent probes: a DFT/TDDFT study. RSC Advances, 2016, 6, 7002-7010.	1.7	28
817	From C₆₀ to Infinity: Large-Scale Quantum Chemistry Calculations of the Heats of Formation of Higher Fullerenes. Journal of the American Chemical Society, 2016, 138, 1420-1429.	6.6	32
818	DFT study of the hydrolysis reaction in atranes and ocanes: the influence of transannular bonding. Journal of Molecular Modeling, 2016, 22, 3.	0.8	7
819	LiCl solvation in N-methyl-acetamide (NMA) as a model for understanding Li⁺binding to an amide plane. Physical Chemistry Chemical Physics, 2016, 18, 4191-4200.	1.3	23
820	The Câ€“H bond dissociation enthalpies in fused N-heterocyclic compounds. Russian Journal of Physical Chemistry A, 2016, 90, 610-621.	0.1	2
821	â€œRate-limited effectâ€•of reverse intersystem crossing process: the key for tuning thermally activated delayed fluorescence lifetime and efficiency roll-off of organic light emitting diodes. Chemical Science, 2016, 7, 4264-4275.	3.7	212

#	Article	IF	Citations
822	An Energetic Guide for Estimating Trifluoromethyl Cation Donor Abilities of Electrophilic Trifluoromethylating Reagents: Computations of Xâ€“CF₃ Bond Heterolytic Dissociation Enthalpies. Journal of Organic Chemistry, 2016, 81, 3119-3126.	1.7	48
823	Exploring the limits of recent exchangeâ€“correlation functionals in modeling lithium/benzene interaction. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	26
824	Computer Modeling of Halogen Bonds and Other Ïƒ-Hole Interactions. Chemical Reviews, 2016, 116, 5155-5187.	23.0	537
825	Hydrogen-atom attack on phenol and toluene is ortho-directed. Physical Chemistry Chemical Physics, 2016, 18, 8625-8636.	1.3	9
826	Theoretical study on the unimolecular decomposition of 2-chlorinated ethyl hydroperoxide. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650008.	1.8	1
827	Intramolecular interactions, isomerization and vibrational frequencies of two paracetamol analogues: A spectroscopic and a computational approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 162, 16-26.	2.0	11
828	The HO2 + (H2O)n + O3 reaction: an overview and recent developments. European Physical Journal D, 2016, 70, 1.	0.6	11
829	Benchmarking semiempirical, Hartreeâ€“Fock, DFT, and MP2 methods against the ionization energies and electron affinities of short- through long-chain [n]acenes and [n]phenacenes. Canadian Journal of Chemistry, 2016, 94, 251-258.	0.6	8
830	Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. Molecular Physics, 2016, 114, 21-33.	0.8	21
831	NIR absorbing Dâ€“Ïâ€“Aâ€“Ïâ€“D structured diketopyrrolopyrroleâ€“dithiafulvalene based small molecule for solution processed organic solar cells. Chemical Communications, 2016, 52, 210-213.	2.2	38
832	Density functional theory is straying from the path toward the exact functional. Science, 2017, 355, 49-52.	6.0	711
833	Can Fluorenone-Based Compounds Emit in the Blue Region? Impact of the Conjugation Length and the Ground-State Aggregation. Chemistry of Materials, 2017, 29, 1695-1707.	3.2	31
834	Efficient modeling of liquid phase photoemission spectra and reorganization energies: Difficult case of multiply charged anions. Journal of Computational Chemistry, 2017, 38, 427-437.	1.5	9
835	Variational Effect and Anharmonic Torsion on Kinetic Modeling for Initiation Reaction of Dimethyl Ether Combustion. Journal of Physical Chemistry A, 2017, 121, 1121-1132.	1.1	12
836	Singularity Correction for Long-Range-Corrected Density Functional Theory with Plane-Wave Basis Sets. Journal of Physical Chemistry A, 2017, 121, 2035-2045.	1.1	1
837	Calculations of solidâ€state ⁴³Ca NMR parameters: A comparison of periodic and cluster approaches and an evaluation of DFT functionals. Journal of Computational Chemistry, 2017, 38, 949-956.	1.5	19
838	Fine tuning phosphorescent properties of platinum complexes via different N -heterocyclic-based CË†NË†N ligands. Journal of Organometallic Chemistry, 2017, 836-837, 26-33.	0.8	7
839	A theoretical study of phosphorescent Cu(I) complexes with 2-(2'quinolyl)imidazole and POP mixed ligands. Organic Electronics, 2017, 45, 9-19.	1.4	13

#	Article	IF	Citations
840	When does a functional correctly describe both the structure and the energy of the transition state?. Journal of Molecular Modeling, 2017, 23, 65.	0.8	5
841	Benchmark study of structural and vibrational properties of scandium clusters. Journal of Molecular Structure, 2017, 1142, 139-147.	1.8	6
842	About the nature of halogen bond interaction under the spatial confinement. Journal of Chemical Physics, 2017, 146, 154304.	1.2	2
843	Comparing the performance of TDâ€DFT and SACâ€CI methods in the description of excited states potential energy surfaces: An excited state proton transfer reaction as case study. Journal of Computational Chemistry, 2017, 38, 1084-1092.	1.5	15
844	Accurate calculations of the noncovalent systems with flat potential energy surfaces: Naphthalene dimer and azulene dimer. Computational and Theoretical Chemistry, 2017, 1112, 52-60.	1.1	4
845	Solid State Separation and Isolation of Tautomers of Fused-Ring Triazolotriazoles. Journal of Organic Chemistry, 2017, 82, 5155-5161.	1.7	14
846	Computational investigation and comparison of hydrogen storage properties of B24N24 and Al24N24 nanocages. International Journal of Hydrogen Energy, 2017, 42, 14166-14180.	3.8	7
847	Theoretical investigation of high-efficiency organic electroluminescent material: HLCT state and hot exciton process. RSC Advances, 2017, 7, 19576-19583.	1.7	48
848	Coupled Cluster and Density Functional Studies of Atomic Fluorine Chemisorption on Coronene as Model Systems for Graphene Fluorination. Journal of Physical Chemistry C, 2017, 121, 14888-14898.	1.5	12
849	Shedding Light on the Accuracy of Optimally Tuned Range-Separated Approximations for Evaluating Oxidation Potentials. Journal of Physical Chemistry A, 2017, 121, 4189-4201.	1.1	14
850	Computational investigation on the large energy gap between the triplet excited-states in acenes. RSC Advances, 2017, 7, 26697-26703.	1.7	26
851	Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. Molecular Physics, 2017, 115, 2315-2372.	0.8	1,401
852	Terahertz investigations on photoisomerisable compounds. Molecular Physics, 2017, 115, 2486-2494.	0.8	2
853	Unification of the W1X and G4(MP2)-6X Composite Protocols. Journal of Chemical Theory and Computation, 2017, 13, 2642-2649.	2.3	27
854	Benchmarking of density functionals for the kinetics and thermodynamics of the hydrolysis of glycosidic bonds catalyzed by glycosidases. International Journal of Quantum Chemistry, 2017, 117, e25409.	1.0	37
855	Can DFT and ab initio methods adequately describe binding energies in strongly interacting C6X6â‹¯C2X Ï€â€“Ï€ complexes?. Chemical Physics, 2017, 493, 12-19.	0.9	7
856	Analysis of Hydrogen Atom Abstraction from Ethylbenzene by an Fe^VO(TAML) Complex. Inorganic Chemistry, 2017, 56, 4347-4356.	1.9	8
857	Theoretical Study on Hydrogenolytic Cleavage of Intermonomer Linkages in Lignin. Journal of Physical Chemistry A, 2017, 121, 2868-2877.	1.1	10

#	Article	IF	Citations
858	A Theoretical Study on Methane Câ€"H Bond Activation by Bare [FeO]^{+/0/â€“}. Journal of Physical Chemistry A, 2017, 121, 3501-3514.	1.1	16
859	Assessment of model chemistries for hydrofluoropolyethers: A DFT/M08â€HX benchmark study. International Journal of Quantum Chemistry, 2017, 117, e25381.	1.0	8
860	Solvatochromic effect in absorption and emission spectra of star-shaped bipolar derivatives of 1,3,5-triazine and carbazole. A time-dependent density functional study. Journal of Molecular Modeling, 2017, 23, 55.	0.8	11
861	TD-DFT benchmark: Excited states of atoms and atomic ions. Computational and Theoretical Chemistry, 2017, 1108, 50-56.	1.1	12
862	Benchmark Study of Density Functional Theory for Neutral Gold Clusters, Au_n (n = 2â€"8). Journal of Physical Chemistry A, 2017, 121, 2410-2419.	1.1	34
863	Thermochemical and Kinetics of CH₃SH + H Reactions: The Sensitivity of Coupling the Low and High-Level Methodologies. Journal of Physical Chemistry A, 2017, 121, 419-428.	1.1	10
864	An appraisal of the hydrogen atom transfer mechanism for the reaction between thiourea derivatives and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mtext /></mml:mrow></mml:msup><mml:mtext>OH</mml:mtext></mml:mrow></mml:math> radical: A case-study of dimethylthiourea and diethylthiourea. Computational and Theoretical Chemistry, 2017, 1101, 83-95.	1.1	13
865	Computational study on Câ€"B homolytic bond dissociation enthalpies of organoboron compounds. New Journal of Chemistry, 2017, 41, 1346-1362.	1.4	12
866	Radical Reaction Control in the AdoMet Radical Enzyme CDG Synthase (QueE): Consolidate, Destabilize, Accelerate. Chemistry - A European Journal, 2017, 23, 953-962.	1.7	10
867	A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. Physical Chemistry Chemical Physics, 2017, 19, 32184-32215.	1.3	1,230
868	Optical Gaps in Pristine and Heavily Doped Silicon Nanocrystals: DFT versus Quantum Monte Carlo Benchmarks. Journal of Chemical Theory and Computation, 2017, 13, 6061-6067.	2.3	11
869	Relevance of the DFT method to study expanded porphyrins with different topologies. Journal of Computational Chemistry, 2017, 38, 2819-2828.	1.5	64
870	Development of a TDDFT-Based Protocol with Local Hybrid Functionals for the Screening of Potential Singlet Fission Chromophores. Journal of Chemical Theory and Computation, 2017, 13, 4984-4996.	2.3	57
871	Speed-Up of the Excited-State Benchmarking: Double-Hybrid Density Functionals as Test Cases. Journal of Chemical Theory and Computation, 2017, 13, 5539-5551.	2.3	33
872	Theoretical study on homolytic Bâ€"B cleavages of diboron(4) compounds. RSC Advances, 2017, 7, 49251-49272.	1.7	8
873	Evaluation of the Factors Impacting the Accuracy of ¹³C NMR Chemical Shift Predictions using Density Functional Theoryâ€"The Advantage of Long-Range Corrected Functionals. Journal of Chemical Theory and Computation, 2017, 13, 5798-5819.	2.3	77
874	Control of Câ€"H Bond Activation by Mo-Oxo Complexes: pK_a or Bond Dissociation Free Energy (BDFE)?. Inorganic Chemistry, 2017, 56, 12319-12327.	1.9	18
875	Ruthenium(II) Polypyridyl Complexes Coordinated Directly to the Pyrrole Backbone of Ï€-Extended Boron Dipyrromethene (Bodipy) Dyes: Synthesis, Characterization, and Spectroscopic and Electrochemical Properties. Inorganic Chemistry, 2017, 56, 10664-10673.	1.9	10

#	Article	IF	Citations
876	Molecular attochemistry in non-polar liquid environments: ultrafast charge migration dynamics through goldâ€“thiolate and goldâ€“selenolate linkages. Physical Chemistry Chemical Physics, 2017, 19, 26679-26696.	1.3	2
877	A simple and efficient protocol for screening boron-dipyrromethene dyes using TD-DFT and an examination of the aryl-meso position. Computational and Theoretical Chemistry, 2017, 1118, 107-114.	1.1	6
878	Is Vitamin A an Antioxidant or a Pro-oxidant?. Journal of Physical Chemistry B, 2017, 121, 9348-9357.	1.2	52
879	Energy Transfer in Microhydrated Uracil, 5-Fluorouracil, and 5-Bromouracil. Journal of Physical Chemistry B, 2017, 121, 8965-8974.	1.2	33
880	Thermochemistry and Kinetics of the Thermal Decomposition of 1â€Chlorohexane. International Journal of Chemical Kinetics, 2017, 49, 743-751.	1.0	2
881	Optimal Tuning of Range-Separated Hybrids for Solvated Molecules with Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 4972-4983.	2.3	18
882	Role of dispersion corrected hybrid GGA class in accurately calculating the bond dissociation energy of carbon halogen bond: A benchmark study. Journal of Molecular Structure, 2017, 1150, 447-458.	1.8	17
883	Modeling Ïƒ-Bond Activations by Nickel(0) Beyond Common Approximations: How Accurately Can We Describe Closed-Shell Oxidative Addition Reactions Mediated by Low-Valent Late 3d Transition Metal?. Journal of Chemical Theory and Computation, 2017, 13, 4841-4853.	2.3	5
884	Theoretical tuning of the singletâ€“triplet energy gap to achieve efficient long-wavelength thermally activated delayed fluorescence emitters: the impact of substituents. Physical Chemistry Chemical Physics, 2017, 19, 21639-21647.	1.3	14
885	Correlation functional in screenedâ€exchange density functional theory procedures. Journal of Computational Chemistry, 2017, 38, 2307-2315.	1.5	11
886	Thermal isomerization of azobenzenes: on the performance of Eyring transition state theory. Journal of Physics Condensed Matter, 2017, 29, 314002.	0.7	19
887	Using non-empirically tuned range-separated functionals with simulated emission bands to model fluorescence lifetimes. Physical Chemistry Chemical Physics, 2017, 19, 21046-21057.	1.3	12
888	Validation of density functionals for pancake-bonded Ï€-dimers; dispersion is not enough. Physical Chemistry Chemical Physics, 2017, 19, 24761-24768.	1.3	32
889	Assessing accuracy of exchange-correlation functionals for electron affinities. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750052.	1.8	1
890	Resolving Discrepancy between Theory and Experiment in 4-Nitrotoluene Oxidation. Journal of Physical Chemistry A, 2017, 121, 6638-6645.	1.1	5
891	Theoretical study of the substituent effect controlling the radiative and non-radiative decay processes of platinum(ii) complexes. Physical Chemistry Chemical Physics, 2017, 19, 23532-23540.	1.3	16
892	Why are GGAs so accurate for reaction kinetics on surfaces? Systematic comparison of hybrid vs. nonhybrid DFT for representative reactions. Journal of Chemical Physics, 2017, 146, 234103.	1.2	11
893	Assessing Excited State Energy Gaps with Time-Dependent Density Functional Theory on Ru(II) Complexes. Journal of Chemical Theory and Computation, 2017, 13, 4123-4145.	2.3	39

#	Article	IF	Citations
894	Atmospheric chemistry of CH₃O: its unimolecular reaction and reactions with H₂O, NH₃, and HF. RSC Advances, 2017, 7, 56211-56219.	1.7	11
895	Ground-State Gas-Phase Structures of Inorganic Molecules Predicted by Density Functional Theory Methods. ACS Omega, 2017, 2, 8373-8387.	1.6	14
896	Chiral ethylene-bridged flavinium salts: the stereoselectivity of flavin-10a-hydroperoxide formation and the effect of substitution on the photochemical properties. Tetrahedron: Asymmetry, 2017, 28, 1780-1791.	1.8	10
897	How Well Can the M06 Suite of Functionals Describe the Electron Densities of Ne, Ne⁶⁺, and Ne⁸⁺?. Journal of Chemical Theory and Computation, 2017, 13, 6068-6077.	2.3	25
898	The Hydrogen Abstraction Reaction H₂S + OH â†' H₂O + SH: Convergent Quantum Mechanical Predictions. Journal of Physical Chemistry A, 2017, 121, 9136-9145.	1.1	11
899	Reaction kinetics of hydrogen abstraction from polycyclic aromatic hydrocarbons by H atoms. Physical Chemistry Chemical Physics, 2017, 19, 30772-30780.	1.3	48
900	Coupled Valence-Bond State Molecular Dynamics Description of an Enzyme-Catalyzed Reaction in a Non-Aqueous Organic Solvent. Journal of Physical Chemistry B, 2017, 121, 7027-7041.	1.2	11
901	Revealing isomerism in sodium-water clusters: Photoionization spectra of Na(H2O)n (n =) Tj ETQq1 1 0.784314 rgBT /O	1.2	6
902	Benchmarking of density functionals for a soft but accurate prediction and assignment of ¹H and ¹³C NMR chemical shifts in organic and biological molecules. Journal of Computational Chemistry, 2017, 38, 87-92.	1.5	28
903	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
904	Stability of the chlorinated derivatives of the DNA/RNA nucleobases, purine and pyrimidine toward radical formation via homolytic Cï£¿Cl bond dissociation. International Journal of Quantum Chemistry, 2017, 117, e25319.	1.0	8
905	The role of hydrogen bonding in the fluorescence quenching of 2,6-bis((E)-2-(benzoxazol-2-yl)vinyl)naphthalene (BBVN) in methanol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 173, 681-686.	2.0	8
906	Benchmarking singlet and triplet excitation energies of molecular semiconductors for singlet fission: Tuning the amount of HF exchange and adjusting local correlation to obtain accurate functionals for singletâ€"triplet gaps. Chemical Physics, 2017, 482, 319-338.	0.9	44
907	Reactivity, vibrational spectroscopy, internal rotation and thermochemical aspects of methylarsine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 171, 383-394.	2.0	9
908	Formation of secondary organic aerosols from the ozonolysis of dihydrofurans. Atmospheric Chemistry and Physics, 2017, 17, 2347-2357.	1.9	8
909	Catalyst Screening through Quantum Chemical Calculations and Microkinetic Modeling: Hydrolysis of Carbon Dioxide. Theoretical Foundations of Chemical Engineering, 2017, 51, 949-960.	0.2	4
910	A theoretical investigation on the neutral Cu(I) phosphorescent complexes with azole-based and phosphine mixed ligand. Molecular Physics, 2018, 116, 898-909.	0.8	3
911	Theoretical study of radiative and nonradiative decay rates for Cu(<scp>i</scp>) complexes with double heteroleptic ligands. Physical Chemistry Chemical Physics, 2018, 20, 9419-9428.	1.3	14

#	Article	IF	Citations
912	Electronic structure and luminescence properties of unique complexes: cyclometalated iridium(<scp>iii</scp>) chelated by o-carboranyl-pyridine ligands. New Journal of Chemistry, 2018, 42, 5955-5966.	1.4	5
913	Hyper Open-Shell Excited Spin States of Transition-Metal Compounds: FeF2, FeF2Â·Â·Â·Ethane, and FeF2Â·Â·Â·Ethylene. Journal of Physical Chemistry A, 2018, 122, 2563-2579.	1.1	12
914	Near infra-red dyes based on pyrene aza-BODIPYs. New Journal of Chemistry, 2018, 42, 5875-5888.	1.4	20
915	Theoretical Investigation of the Gas-Phase S_N2 Reactions of Anionic and Neutral Nucleophiles with Chloramines. Journal of Physical Chemistry A, 2018, 122, 3045-3056.	1.1	4
916	Reactivity of cycloparaphenylenes: Studying the possible growth of single-walled carbon nanotubes with DFT methods. Chemical Physics Letters, 2018, 697, 17-22.	1.2	2
917	How the Connectivity of Methoxy Substituents Influences the Photovoltaic Properties of Dissymmetric Core Materials: A Theoretical Study on FDT. Journal of Physical Chemistry C, 2018, 122, 8804-8813.	1.5	11
918	Interligand Charge-Transfer Interactions in Electroactive Coordination Frameworks Based on N,Nâ€²-Dicyanoquinonediimine (DCNQI). Inorganic Chemistry, 2018, 57, 9766-9774.	1.9	9
919	The Electronic Structure and Spectra of Triphenylamines Functionalized by Phenylethynyl Groups. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2018, 124, 57-64.	0.2	1
920	Theoretical kinetics study of the reactions CHClBrâ€¯+â€¯HBrâ€¯â‡„â€¯CH2ClBrâ€¯+â€¯Br, CCl2Brâ€¯+â€¯HBrâ€¯â‡„â€¯CHCl2Brâ€¯+â€¯B CClBr2â€¯+â€¯HBrâ€¯â‡„â€¯CHClBr2â€¯+â€¯Br. Chemical Physics Letters, 2018, 696, 79-85.	1.2	0
921	Modeling the Reactions Catalyzed by Coenzyme B₁₂ Dependent Enzymes: Accuracy and Cost-Quality Balance. Journal of Physical Chemistry A, 2018, 122, 1747-1755.	1.1	11
922	Theoretical Prediction of Activation Free Energies of Various Hydride Self-Exchange Reactions in Acetonitrile at 298 K. ACS Omega, 2018, 3, 872-885.	1.6	16
923	Multiscale modeling of enzymes: QMâ€cluster, QM/MM, and QM/MM/MD: A tutorial review. International Journal of Quantum Chemistry, 2018, 118, e25558.	1.0	106
924	B97-3c: A revised low-cost variant of the B97-D density functional method. Journal of Chemical Physics, 2018, 148, 064104.	1.2	400
925	What Happens Without Nickel? Cyclization Reactions of Ethylene with Ethanedithial and Related Molecules. Journal of Computational Chemistry, 2018, 39, 1158-1167.	1.5	0
926	Introducing Membrane Transport Energy into the Design of Sustainable Chemicals against Cytotoxicity. ACS Sustainable Chemistry and Engineering, 2018, 6, 2055-2061.	3.2	2
927	Rational Density Functional Selection Using Game Theory. Journal of Chemical Information and Modeling, 2018, 58, 61-67.	2.5	20
928	Isomerization patterns and proton transfer in ionic liquids constituents as probed by ab-initio computation. Journal of Molecular Liquids, 2018, 249, 1075-1082.	2.3	9
929	A Theoretical study on the degradation of 2-mercaptobenzothiazole and 2-mercaptobenzimidazole by OH in vacuo and aqueous media. Computational and Theoretical Chemistry, 2018, 1125, 112-127.	1.1	5

#	Article	IF	Citations
930	How are the charge transfer descriptors affected by the quality of the underpinning electronic density?. Journal of Computational Chemistry, 2018, 39, 735-742.	1.5	22
931	Theoretical insight into the regioselective ring-expansions of bicyclic aziridinium ions. Organic and Biomolecular Chemistry, 2018, 16, 796-806.	1.5	16
932	Through-Space Intervalence Charge Transfer as a Mechanism for Charge Delocalization in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2018, 140, 6622-6630.	6.6	120
933	Transition metal hydrides MH+/0/â^' (Mâ€¯=â€¯Scâ^'Zn): Benchmark study and periodic trends. Computational and Theoretical Chemistry, 2018, 1134, 15-21.	1.1	2
934	Enantiopure Schiff bases of amino acid phenylhydrazides: impact of the hydrazide function on their structures and properties. New Journal of Chemistry, 2018, 42, 6389-6398.	1.4	11
935	How Accurate Is Density Functional Theory at Predicting Dipole Moments? An Assessment Using a New Database of 200 Benchmark Values. Journal of Chemical Theory and Computation, 2018, 14, 1969-1981.	2.3	180
936	Electronic structures and photophysical properties of phosphorescent platinum (II) complexes with tridentate C^N*N cyclometalated ligands. Applied Organometallic Chemistry, 2018, 32, e3929.	1.7	8
937	Benzimidazobenzothiazole-based highly-efficient thermally activated delayed fluorescence emitters for organic light-emitting diodes: A quantum-chemical TD-DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 192, 297-303.	2.0	5
938	Thermodynamics of aqueous perfluorooctanoic acid (PFOA) and 4,8-dioxa-3H-perfluorononanoic acid (DONA) from DFT calculations: Insights into degradation initiation. Chemosphere, 2018, 193, 1063-1070.	4.2	20
939	Shortfall of B3LYP in Reproducing NMR J_{CH} Couplings in Some Isomeric Epoxy Structures with Strong Stereoelectronic Effects: A Benchmark Study on DFT Functionals. ChemPhysChem, 2018, 19, 631-642.	1.0	12
940	Revealing the Unique Properties of Platinum(II) Complexes with Bidentate Bis(o -carborane) Ligands. European Journal of Inorganic Chemistry, 2018, 2018, 99-108.	1.0	6
941	Spectroscopic, electronic and computational properties of a mixed tetrachalcogenafulvalene and its charge transfer complex. Journal of Materials Chemistry C, 2018, 6, 1092-1104.	2.7	11
942	â€œTradeâ€Offâ€•Hidden in Condensed State Solvation: Multiradiative Channels Design for Highly Efficient Solutionâ€Processed Purely Organic Electroluminescence at High Brightness. Advanced Functional Materials, 2018, 28, 1704927.	7.8	105
943	Benchmarking of DFT functionals for the kinetics and mechanisms of atmospheric addition reactions of OH radicals with phenyl and substituted phenylâ€based organic pollutants. International Journal of Quantum Chemistry, 2018, 118, e25533.	1.0	14
944	On the Performance of Hybrid Functionals for Nonâ€linear Optical Properties and Electronic Excitations in Chiral Molecular Crystals: The Case of Butterflyâ€Shaped Dicinnamalacetone. ChemPhysChem, 2018, 19, 82-92.	1.0	9
945	Reactivity Indices of Polyaromatic Hydrocarbons for the Radical Reactions of Coke Layer Formation on the Visbreaking of Hydrocarbon Raw Materials. Solid Fuel Chemistry, 2018, 52, 382-386.	0.2	0
946	Factors governing when a metal-bound water is deprotonated in proteins. Physical Chemistry Chemical Physics, 2018, 20, 29625-29636.	1.3	7
947	An efficient protocol for computing the pKa of Zn-bound water. Physical Chemistry Chemical Physics, 2018, 20, 29637-29647.	1.3	10

#	Article	IF	Citations
948	3. Structure and Theory. , 2018, , 51-166.		0
949	How Pb²⁺ Binds and Modulates Properties of Ca²⁺-Signaling Proteins. Inorganic Chemistry, 2018, 57, 14798-14809.	1.9	35
950	Importance of Chromophore Rigidity on the Efficiency of Blue Thermally Activated Delayed Fluorescence Emitters. Journal of Physical Chemistry C, 2018, 122, 28564-28575.	1.5	35
951	QM/MM Study of the Reaction Mechanism of the Dehydratase Domain from Mammalian Fatty Acid Synthase. ACS Catalysis, 2018, 8, 10267-10278.	5.5	34
952	Umbrella inversion and structure of phosphorus-containing compounds: A quantum chemical study. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850042.	1.8	7
953	Naphthalimide-Based Fluorescent Dyes: Impact of Extension of Ï€-Conjugation and Introduction of an Electron-Donating Moiety on the Photophysical Properties. Bulletin of the Chemical Society of Japan, 2018, 91, 1506-1514.	2.0	1
954	Uncontracted core Pople basis sets in vibrational frequency calculations. International Journal of Quantum Chemistry, 2018, 118, e25761.	1.0	4
955	Solid State Selection between Nearly Isoenergetic Tautomeric Forms Driven by Right Hydrogen-Bonding Pairing. Crystal Growth and Design, 2018, 18, 6293-6301.	1.4	7
956	Stability and Electronic Properties of Rocksalt (CdO)_n, (SrO)_n, and (BaO)_n Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 25021-25034.	1.5	6
957	Lessons from the Spin-Polarization/Spin-Contamination Dilemma of Transition-Metal Hyperfine Couplings for the Construction of Exchange-Correlation Functionals. Journal of Chemical Theory and Computation, 2018, 14, 5653-5672.	2.3	35
958	Performance of density functional theory for describing heteroâ€metallic activeâ€site motifs for methaneâ€toâ€methanol conversion in metalâ€exchanged zeolites. Journal of Computational Chemistry, 2018, 39, 2667-2678.	1.5	8
959	The Energetic Viability of Î”1-Piperideine Dimerization in Lysine-derived Alkaloid Biosynthesis. Metabolites, 2018, 8, 48.	1.3	11
960	Delocalization Errors in Density Functional Theory Are Essentially Quadratic in Fractional Occupation Number. Journal of Physical Chemistry Letters, 2018, 9, 6280-6288.	2.1	71
961	Theoretical insight into structural and electronic properties of cationic Scn+ (n=2-13): A benchmark study. Solid State Sciences, 2018, 86, 60-68.	1.5	3
962	Mechanistic Studies of a Flavin Monooxygenase: Sulfur Oxidation of Dibenzothiophenes by DszC. ACS Catalysis, 2018, 8, 9298-9311.	5.5	17
963	Why the lowest electronic excitations of rhodamines are overestimated by timeâ€dependent density functional theory. International Journal of Quantum Chemistry, 2018, 118, e25780.	1.0	31
964	Exploring the Limitation of Molecular Water Oxidation Catalysts. Journal of Physical Chemistry C, 2018, 122, 12404-12412.	1.5	37
965	Exploring conformational preferences of alanine tetrapeptide by CCSD(T), MP2, and dispersion-corrected DFT methods. Chemical Physics Letters, 2018, 702, 69-75.	1.2	12

#	Article	IF	Citations
966	Benchmarking DFT methods on linear and nonlinear electric properties of spatially confined molecules. International Journal of Quantum Chemistry, 2018, 118, e25666.	1.0	14
967	When Hartree-Fock exchange admixture lowers DFT-predicted barrier heights: Natural bond orbital analyses and implications for catalysis. Journal of Chemical Physics, 2018, 148, 244106.	1.2	25
968	First-principles calculations of oxidation potentials of electrolytes in lithiumâ€“sulfur batteries and their variations with changes in environment. Physical Chemistry Chemical Physics, 2018, 20, 18811-18827.	1.3	8
969	Theoretical investigation of Banert cascade reaction. Royal Society Open Science, 2018, 5, 171075.	1.1	7
970	Reaction of CO₂ with Atomic Transition Metal M^{+/0/â€“} Ions: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 5848-5860.	1.1	10
971	DFT/TDDFT insight into the impact of ring size of the NHC chelating unit of high effective phosphorescent Platinum (II) complexes. Applied Organometallic Chemistry, 2018, 32, e4467.	1.7	10
972	Access to 3-aminobenzothiophenes and 3-aminothiophenes fused to 5-membered heteroaromatic rings through 6Ï€-electrocyclization reaction of keteniminium salts. Tetrahedron Letters, 2018, 59, 3242-3248.	0.7	17
973	CBS extrapolation in electronic structure pushed to the end: a revival of minimal and sub-minimal basis sets. Physical Chemistry Chemical Physics, 2018, 20, 22084-22098.	1.3	25
974	Comparison of the Transition Dipole Moments Calculated by TDDFT with High Level Wave Function Theory. Journal of Chemical Theory and Computation, 2018, 14, 5303-5309.	2.3	18
975	A theoretical study of the thermal stability of the FS(O2)OSO2 radical and the recombination kinetics with the FSO3 radical. Computational and Theoretical Chemistry, 2018, 1123, 87-95.	1.1	1
976	Non-orthogonal configuration interaction with single substitutions for the calculation of core-excited states. Journal of Chemical Physics, 2018, 149, 044116.	1.2	44
977	Semi-empirical or non-empirical double-hybrid density functionals: which are more robust?. Physical Chemistry Chemical Physics, 2018, 20, 23175-23194.	1.3	102
978	How accurate are static polarizability predictions from density functional theory? An assessment over 132 species at equilibrium geometry. Physical Chemistry Chemical Physics, 2018, 20, 19800-19810.	1.3	94
979	Design of a Novel Series of Donorâ€“Acceptor Frameworks via Superalkaliâ€“Superhalogen Assemblage to Improve the Nonlinear Optical Responses. Inorganic Chemistry, 2018, 57, 9335-9347.	1.9	37
980	Formulation of Small Test Sets Using Large Test Sets for Efficient Assessment of Quantum Chemistry Methods. Journal of Chemical Theory and Computation, 2018, 14, 4254-4262.	2.3	25
981	The influence of the structural variations of the fused electron rich-electron deficient unit in the Ï€-spacer of A-D-Ï€-D-A organic dyes on the efficiency of dye-sensitized solar cells: A computational study. Organic Electronics, 2018, 62, 43-55.	1.4	13
982	MVO-10: A Gas-Phase Oxide Benchmark for Localization/Delocalization in Mixed-Valence Systems. Journal of Chemical Theory and Computation, 2018, 14, 3512-3523.	2.3	20
983	Accuracy of TD-DFT Geometries: A Fresh Look. Journal of Chemical Theory and Computation, 2018, 14, 3715-3727.	2.3	74

#	Article	IF	Citations
984	Computational Tale of Two Enzymes: Glycerol Dehydration With or Without B₁₂. Journal of the American Chemical Society, 2018, 140, 8487-8496.	6.6	24
985	Ab initio photodynamics of model EUV photoresists. Chemical Physics, 2018, 515, 221-230.	0.9	9
986	Theoretical Investigation of the Reaction of Pyrene Formation from Fluoranthene. Journal of Physical Chemistry A, 2019, 123, 7491-7498.	1.1	4
987	Does Involving Additional Linker Always Increase the Efficiency of an Organic Dye for p-Type Dye-Sensitized Solar Cells?. ACS Applied Energy Materials, 2019, 2, 6341-6347.	2.5	33
988	Statistically representative databases for density functional theory via data science. Physical Chemistry Chemical Physics, 2019, 21, 19092-19103.	1.3	20
989	Theoretical insights into the effect of ligands on platinum(ii) complexes with a bidentate bis(o-carborane) ligand structure. Photochemical and Photobiological Sciences, 2019, 18, 2421-2429.	1.6	3
990	Tautomerism in Azo and Azomethyne Dyes: When and If Theory Meets Experiment. Molecules, 2019, 24, 2252.	1.7	31
991	Importance of Conformational Change in Excited States for Efficient Thermally Activated Delayed Fluorescence. Journal of Physical Chemistry C, 2019, 123, 19322-19332.	1.5	26
992	Cost-effective density functional theory (DFT) calculations of equilibrium isotopic fractionation in large organic molecules. Physical Chemistry Chemical Physics, 2019, 21, 17555-17570.	1.3	11
993	G4(MP2)-XK: A Variant of the G4(MP2)-6X Composite Method with Expanded Applicability for Main-Group Elements up to Radon. Journal of Chemical Theory and Computation, 2019, 15, 4478-4484.	2.3	34
994	Electronic structure and optical properties of isolated and TiO₂â€grafted free base porphyrins for water oxidation: A challenging test case for DFT and TDâ€DFT. Journal of Computational Chemistry, 2019, 40, 2530-2538.	1.5	9
995	Accurate Binding Energies for Lithium Polysulfides and Assessment of Density Functionals for Lithiumâ€“Sulfur Battery Research. Journal of Physical Chemistry C, 2019, 123, 20737-20747.	1.5	34
996	Computational Study of Glycerol Binding within the Active Site of Coenzyme B₁₂-Dependent Diol Dehydratase. Journal of Physical Chemistry B, 2019, 123, 6178-6187.	1.2	6
997	Chemical Kinetics of Hydrogen Atom Abstraction from Propargyl Sites by Hydrogen and Hydroxy Radicals. International Journal of Molecular Sciences, 2019, 20, 3227.	1.8	6
998	Selfâ€Assemble and Inâ€Situ Formation of Laponite RDSâ€Decorated dâ€Ti₃C₂T_x Hybrids for Application in Lithiumâ€ion Battery. ChemistrySelect, 2019, 4, 10694-10700.	0.7	5
999	Stability of â€œNo-Pair Ferromagneticâ€•Lithium Clusters. Journal of Physical Chemistry A, 2019, 123, 9721-9728.	1.1	3
1000	Application of quantum chemical methods in polymer chemistry. International Reviews in Physical Chemistry, 2019, 38, 343-403.	0.9	22
1001	A DFT mechanistic and kinetic study on the reaction of phloroglucinol with ^{â€¢}OH in different media: Hydrogen atom transfer versus oxidation. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950017.	1.8	6

#	Article	IF	Citations
1002	A DFT mechanistic, thermodynamic and kinetic study on the reaction of 1, 3, 5-trihydroxybenzene and 2, 4, 6-trihydroxyacetophenone with ^{â€¢}OOH in different media. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950023.	1.8	5
1003	Theoretical study of gallium nitride nanocage as a carrier for 5-fluorouracil anticancer drug. Journal of Molecular Modeling, 2019, 25, 265.	0.8	17
1004	Exploring the optoelectronic and charge transport properties of Pechmann dyes as efficient OLED materials. Optik, 2019, 197, 163200.	1.4	14
1005	Assessment of pK_a Determination for Monocarboxylic Acids with an Accurate Theoretical Composite Method: G4CEP. Journal of Physical Chemistry A, 2019, 123, 8314-8320.	1.1	10
1006	Computational investigation on the reaction of dimethyl ether with nitric dioxide. I. Underlying mechanism and accurate energetics. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	4
1007	Achieving Conformational Control in Room-Temperature Phosphorescence and Thermally Activated Delayed Fluorescence Emitters by Functionalization of the Central Core. Journal of Physical Chemistry C, 2019, 123, 26536-26546.	1.5	21
1008	New Insight into an Old Problem: Analysis, Interpretation, and Theoretical Modeling of the Absorption and Magnetic Circular Dichroism Spectra of Monomeric and Dimeric Zinc Phthalocyanine Cation Radical. Inorganic Chemistry, 2019, 58, 14120-14135.	1.9	17
1009	Kinetics and mechanism of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si18.svg"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CH</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> with <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si19.svg"><mml:mrow><mml:msub><mml:mrow><mml:mtext>H</mml:mtext></mml:mrow></mml:msub></mml:mrow></mml:math>. Chemical Physics Letters, 2019, 734, 136699.	1.2	1
1010	Benchmark DFT studies on Câ€“CN homolytic cleavage and screening the substitution effect on bond dissociation energy. Journal of Molecular Modeling, 2019, 25, 47.	0.8	18
1011	Assessment of a composite method based on selected density functional theory methods and complete basis set extrapolation formulas. International Journal of Quantum Chemistry, 2019, 119, e25892.	1.0	6
1012	A Ru(II)-p-cymene compound bearing naproxen-pyridineamide. Synthesis, spectroscopic studies, computational analysis and in vitro anticancer activity against lung cells compared to Ru(II)-p-cymene-naproxen and the corresponding drug ligands. Inorganica Chimica Acta, 2019, 489, 27-38.	1.2	12
1013	Proton transfer from pinene stabilizes water clusters. Physical Chemistry Chemical Physics, 2019, 21, 13925-13933.	1.3	5
1014	Reassessment of the Mechanisms of Thermal Câ€“H Bond Activation of Methane by Cationic Magnesium Oxides: A Critical Evaluation of the Suitability of Different Density Functionals. ChemPhysChem, 2019, 20, 1812-1821.	1.0	5
1015	Benchmark of Density Functionals for the Calculation of the Redox Potential of Fe3+/Fe2+ Within Protein Coordination Shells. Frontiers in Chemistry, 2019, 7, 391.	1.8	14
1016	Minimally Empirical Double-Hybrid Functionals Trained against the GMTKN55 Database: revDSD-PBEP86-D4, revDOD-PBE-D4, and DOD-SCAN-D4. Journal of Physical Chemistry A, 2019, 123, 5129-5143.	1.1	262
1017	Design of a novel series of small molecule donors for application in organic solar cells. Solar Energy, 2019, 186, 72-83.	2.9	14
1018	New particle formation from the reactions of ozone with indene and styrene. Physical Chemistry Chemical Physics, 2019, 21, 11214-11225.	1.3	8
1019	Clean and Efficient Transformation of CO₂ to Isocyanic Acid: The Important Role of Triatomic Cation ScNH⁺. Journal of Physical Chemistry A, 2019, 123, 5762-5767.	1.1	7

#	Article	IF	Citations
1020	Theoretical insight into the photodeactivation pathway of the tetradentate Pt (II) complex with different inductive substituents. Applied Organometallic Chemistry, 2019, 33, e4879.	1.7	7
1021	Long-range screened hybrid-functional theory satisfying the local-density linear response. Physical Review A, 2019, 99, .	1.0	16
1022	A theoretical study on one-electron redox potentials of organotrifluoroborate anions. New Journal of Chemistry, 2019, 43, 8590-8605.	1.4	0
1023	On the origin of the difference between type A and type B skeletal isomerization of alkenes catalyzed by zeolites: The crucial input of ab initio molecular dynamics. Journal of Catalysis, 2019, 373, 361-373.	3.1	38
1024	Thermochemistry and Kinetics of the Thermal Degradation of 2-Methoxyethanol as Possible Biofuel Additives. Scientific Reports, 2019, 9, 4535.	1.6	20
1025	Basis Set Effects in the Description of the Cl-O Bond in ClO and XClO/ClOX Isomers (Xâ€‰=â€‰H, O, and Cl) Using DFT and CCSD(T) Methods. Journal of Chemistry, 2019, 2019, 1-23.	0.9	5
1026	Evaluation of the antioxidant potential of myricetin 3-O-Î±-L-rhamnopyranoside and myricetin 4â€²-O-Î±-L-rhamnopyranoside through a computational study. Journal of Molecular Modeling, 2019, 25, 89.	0.8	37
1027	Theoretical modeling of pKa's of thiol compounds in aqueous solution. New Journal of Chemistry, 2019, 43, 5239-5254.	1.4	15
1028	Chiral arylideneaminoimidazolidin-4-ones: green synthesis and isomerisation mechanism in solution. New Journal of Chemistry, 2019, 43, 4777-4786.	1.4	1
1029	Cyano substitution effect on the emission quantum efficiency in stilbene derivatives: A computational study. Organic Electronics, 2019, 68, 264-270.	1.4	13
1030	Shock wave and modelling study of the dissociation pathways of (C₂F₅)₃N. Physical Chemistry Chemical Physics, 2019, 21, 9785-9792.	1.3	3
1031	Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchangeâ€“Correlation Functionals: The MOBH35 Benchmark Database. Journal of Physical Chemistry A, 2019, 123, 3761-3781.	1.1	104
1032	A quantum chemical study of the effect of substituents in governing the strength of the Sâ€“F bonds of sulfenyl-type fluorides toward homolytic dissociation and fluorine atom transfer. Chemical Data Collections, 2019, 20, 100186.	1.1	5
1033	Theoretical Insights Into Thermal Self-Initiation Reactions of Acrylates. , 2019, , 99-134.		1
1034	Polymers, Polymerization Reactions, and Computational Quantum Chemistry. , 2019, , 1-16.		3
1035	Balancing charge-transfer strength and triplet states for deep-blue thermally activated delayed fluorescence with an unconventional electron rich dibenzothiophene acceptor. Journal of Materials Chemistry C, 2019, 7, 13224-13234.	2.7	52
1036	Some observations on the performance of the most recent exchange-correlation functionals for the large and chemically diverse GMTKN55 benchmark. AIP Conference Proceedings, 2019, , .	0.3	15
1037	Radical Stabilization Energies for Enzyme Engineering: Tackling the Substrate Scope of the Radical Enzyme QueE. Journal of Chemical Information and Modeling, 2019, 59, 5111-5125.	2.5	7

#	Article	IF	Citations
1038	Fine Structural Tuning of Thieno[3,2-b] Pyrrole Donor for Designing Banana-Shaped Semiconductors Relevant to Organic Field Effect Transistors. Journal of Chemical Information and Modeling, 2019, 59, 1930-1945.	2.5	16
1039	Computational Study of the Reaction of Dimethyl Ether with Nitric Oxide. Mechanism and Kinetic Modeling. Journal of Physical Chemistry A, 2019, 123, 26-36.	1.1	6
1040	The DFT study on Rhâ€“C bond dissociation enthalpies of (iminoacyl)rhodium(III)hydride and (iminoacyl)rhodium(III)alkyl. Tetrahedron Letters, 2019, 60, 310-321.	0.7	4
1041	Simultaneous Prediction of the Energies of Q_x and Q_y Bands and Intramolecular Charge-Transfer Transitions in Benzoannulated and Non-Peripherally Substituted Metal-Free Phthalocyanines and Their Analogues: No Standard TDDFT Silver Bullet Yet. Journal of Physical Chemistry A, 2019, 123, 132-152.	1.1	22
1042	Benchmark study of popular density functionals for calculating binding energies of threeâ€center twoâ€electron bonds. Journal of Computational Chemistry, 2019, 40, 657-670.	1.5	11
1043	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. Journal of Physical Chemistry A, 2019, 123, 517-536.	1.1	13
1044	Hydrogen Abstraction Reaction H2Se + OH â†' H2O + SeH: Comparison with the Analogous Hydrogen Sulfide and Water Reactions. Inorganic Chemistry, 2019, 58, 2069-2079.	1.9	2
1045	Computational discovery of the strongest base: Diethynylborazine dianion. Chemical Physics Letters, 2019, 714, 65-68.	1.2	0
1046	Performance of DFT for C₆₀ Isomerization Energies: A Noticeable Exception to Jacobâ€™s Ladder. Journal of Physical Chemistry A, 2019, 123, 257-266.	1.1	19
1047	Performance of time-dependent density functional theory on twisted intramolecular charge transfer state of emerging visible light photoswitches. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 371, 336-340.	2.0	9
1048	A theoretical investigation on the thermally activated delayed fluorescence characteristics of the isomers of DTCBPy. Journal of Molecular Graphics and Modelling, 2019, 86, 125-131.	1.3	5
1049	Density functional theory study of the oxidation reaction in the gas and aqueous phase of allyl methyl disulfide with hydroxyl radical. Structural Chemistry, 2019, 30, 237-245.	1.0	12
1050	A highly active copper-based metal-organic framework catalyst for a friedelâ€“crafts alkylation in the synthesis of bis(indolyl)methanes under ultrasound irradiation. Arabian Journal of Chemistry, 2020, 13, 1377-1385.	2.3	10
1051	Decomposition kinetics of perfluorinated sulfonic acids. Chemosphere, 2020, 238, 124615.	4.2	55
1052	The effect of molecular structure on the properties of quinoxaline-based molecules for OLED applications. Dyes and Pigments, 2020, 173, 108008.	2.0	34
1053	Theoretical studies on chiral formamide-mediated asymmetric allylation of aldimines. Journal of the Iranian Chemical Society, 2020, 17, 623-630.	1.2	0
1054	Benchmark approach to search of costâ€effective and accurate density functional for homolytic cleavage of Câ€Mg bond of Grignard reagent. International Journal of Quantum Chemistry, 2020, 120, e26106.	1.0	4
1055	Elucidation of the Mechanism of Silverâ€Catalyzed Inverse Electronâ€Demand Dielsâ€Alder (IEDDA) Reaction of 1,2â€Diazines and Siloxy Alkynes. ChemCatChem, 2020, 12, 366-372.	1.8	3

#	Article	IF	Citations
1056	Accurate theoretical prediction of optical properties of BODIPY dyes. International Journal of Quantum Chemistry, 2020, 120, e26159.	1.0	12
1057	Theoretical insights into the effect of pristine, doped and hole graphene on the overall performance of dye-sensitized solar cells. Inorganic Chemistry Frontiers, 2020, 7, 157-168.	3.0	9
1058	Benchmark study of DFT and composite methods for bond dissociation energies in argon compounds. Chemical Physics, 2020, 531, 110676.	0.9	8
1059	Substitution effect on luminescent property of thermally activated delayed fluorescence molecule with aggregation induced emission: A QM/MM study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 229, 117964.	2.0	15
1060	Highly efficient blue-emitting of bis-cyclometalated tetravalent platinum (IV) complexes: A theoretical study. Inorganica Chimica Acta, 2020, 501, 119269.	1.2	4
1061	Phototautomerism of triazolo-triazole scaffold. Journal of Molecular Structure, 2020, 1203, 127368.	1.8	4
1062	Density Functional Theory as a Data Science. Chemical Record, 2020, 20, 618-639.	2.9	9
1063	Empirical Doubleâ€Hybrid Density Functional Theory: A â€˜Third Wayâ€™ in Between WFT and DFT. Israel Journal of Chemistry, 2020, 60, 787-804.	1.0	129
1064	The nonlinear optical properties of acyclic triarylamine-conjugated dimethyl diethynylfumarate and its two cyclic Pechmann dyes derivatives: A theoretical study. Optik, 2020, 207, 163895.	1.4	4
1065	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. Journal of Computational Chemistry, 2020, 41, 328-339.	1.5	13
1066	Self-Consistent Implementation of Hybrid Functionals with Local Range Separation. Journal of Chemical Theory and Computation, 2020, 16, 953-963.	2.3	19
1067	Evaluation of Single-Reference DFT-Based Approaches for the Calculation of Spectroscopic Signatures of Excited States Involved in Singlet Fission. Journal of Physical Chemistry A, 2020, 124, 8446-8460.	1.1	10
1068	Defective Carbon Nanocone as an Anode Material for Lithium-Ion Batteries. ACS Applied Energy Materials, 2020, 3, 11463-11469.	2.5	17
1069	Tautomeric and conformational switching in a new versatile N-rich heterocyclic ligand. Dalton Transactions, 2020, 49, 14452-14462.	1.6	7
1070	Twisted-Planar-Twisted expanded porphyrinoid dimer as a rudimentary reaction-based methanol indicator. Nature Communications, 2020, 11, 5289.	5.8	20
1071	Selectivity control in thiolâ€“yne click reactions via visible light induced associative electron upconversion. Chemical Science, 2020, 11, 10061-10070.	3.7	47
1072	The role of potential energy surface in quantum mechanical tunneling: A computational perspective. Computational and Theoretical Chemistry, 2020, 1187, 112920.	1.1	1
1073	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. Journal of Chemical Theory and Computation, 2020, 16, 7413-7430.	2.3	12

#	Article	IF	Citations
1074	Lithium oxidation and electrolyte decomposition at Li-metal/liquid electrolyte interfaces. Journal of Materials Chemistry A, 2020, 8, 17036-17055.	5.2	28
1075	Efficient strategies for improving the performance of EDOT derivatives and TPA derivatives-based hole transport materials for perovskite solar cells. Solar Energy, 2020, 208, 10-19.	2.9	14
1076	Photophysical, kinetic and thermodynamic study of one-component Type II thioxanthone acetic acid photoinitiators. European Polymer Journal, 2020, 136, 109909.	2.6	19
1077	Heats of formation for aluminium compounds with EnAt1 and EnAt2. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	4
1078	Benchmark study of density functionals for the insertions of olefin and polar monomers catalyzed by Î±â€“diimine palladium complexes. Computational and Theoretical Chemistry, 2020, 1187, 112942.	1.1	3
1079	Triangulenium dyes: the comprehensive photo-absorption and emission story of a versatile family of chromophores. Physical Chemistry Chemical Physics, 2020, 22, 20673-20684.	1.3	5
1080	Solid-State Effect Induced Thermally Activated Delayed Fluorescence with Tunable Emission: A Multiscale Study. Journal of Physical Chemistry A, 2020, 124, 8540-8550.	1.1	18
1081	Accuracy of intermolecular interaction energies, particularly those of hetero-atom containing molecules obtained by DFT calculations with Grimme's D2, D3 and D3BJ dispersion corrections. Physical Chemistry Chemical Physics, 2020, 22, 22508-22519.	1.3	68
1082	Calculated Reduction Potentials of Electrolyte Species in Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2020, 124, 20654-20670.	1.5	18
1083	Tuning Optical Properties by Controlled Aggregation: Electroluminescence Assisted by Thermallyâ€Activated Delayed Fluorescence from Thin Films of Crystalline Chromophores. Chemistry - A European Journal, 2020, 26, 17016-17020.	1.7	25
1084	The electronic spectrum of AgI2. Ab initio benchmark CASSCFÂ+ÂAveraged Coupled Pair Functional studies on the ligand-field states including spin-orbit couplings. Journal of Molecular Spectroscopy, 2020, 373, 111355.	0.4	2
1085	Canonical and DLPNO-Based Composite Wavefunction Methods Parametrized against Large and Chemically Diverse Training Sets. 2: Correlation-Consistent Basis Sets, Coreâ€“Valence Correlation, and F12 Alternatives. Journal of Chemical Theory and Computation, 2020, 16, 7507-7524.	2.3	19
1086	New Perspectives in the Noble Gas Chemistry Opened by Electrophilic Anions. Frontiers in Chemistry, 2020, 8, 580295.	1.8	6
1087	On the Regioselectivity of the Gouldâ€“Jacobs Reaction: Gasâ€Phase Versus Solutionâ€Phase Thermolysis. European Journal of Organic Chemistry, 2020, 2020, 7051-7061.	1.2	5
1088	Third-Order MÃ¸llerâ€“Plesset Theory Made More Useful? The Role of Density Functional Theory Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 7473-7489.	2.3	27
1089	The one-electron self-interaction error in 74 density functional approximations: a case study on hydrogenic mono- and dinuclear systems. Physical Chemistry Chemical Physics, 2020, 22, 15805-15830.	1.3	27
1090	Sulforaphane: A natural product against reactive oxygen species. Computational and Theoretical Chemistry, 2020, 1183, 112850.	1.1	9
1091	Electron Spin Densities and Density Functional Approximations: Open-Shell Polycyclic Aromatic Hydrocarbons as Case Study. Journal of Chemical Theory and Computation, 2020, 16, 3567-3577.	2.3	20

#	Article	IF	Citations
1092	Substituted Benzothietes: Synthesis and a Quantum Chemical Investigation of Their Cycloreversion Properties. Organic Letters, 2020, 22, 4255-4260.	2.4	1
1093	Simulation of the environmental degradation of diuron (herbicide) using electrochemistry coupled to high resolution mass spectrometry. Electrochimica Acta, 2020, 352, 136485.	2.6	18
1094	Chiral thermally activated delayed fluorescence emitters with dual conformations based on a pair of enantiomeric donors containing asymmetric carbons. Dyes and Pigments, 2020, 178, 108336.	2.0	10
1095	The devil in the details: A tutorial review on some undervalued aspects of density functional theory calculations. International Journal of Quantum Chemistry, 2020, 120, e26332.	1.0	63
1096	Heavy atom tunnelling on XeF₆ pseudorotation. Physical Chemistry Chemical Physics, 2020, 22, 17725-17730.	1.3	7
1097	Using electronegativity and hardness to test density functionals. Journal of Chemical Physics, 2020, 152, 244113.	1.2	5
1098	High firstâ€hyperpolarizabilities of thiobarbituric acid derivativeâ€based donorâ€Ï€â€acceptor nonlinear opticalâ€phores: Multiple theoretical investigations of substituents and conjugated bridges effect. International Journal of Quantum Chemistry, 2020, 120, e26176.	1.0	7
1099	Degradation Mechanisms and Substituent Effects of N-Chloro-Î±-Amino Acids: A Computational Study. Environmental Science & Technology, 2020, 54, 2635-2645.	4.6	18
1100	On interaction of arginine, cysteine and guanine with a nano-TiO2 cluster. Computational Biology and Chemistry, 2020, 86, 107236.	1.1	4
1101	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
1102	Electrocatalytic Hydrogen Evolution and Oxidation with Rhenium Tris(thiolate) Complexes: A Competition between Rhenium and Sulfur for Electrons and Protons. ACS Catalysis, 2020, 10, 3778-3789.	5.5	22
1103	Quantum chemical and kinetic study of the CCl2â€¯+â€¯HClâ€¯â†’â€¯CHCl3 insertion reaction. Computational and Theoretical Chemistry, 2020, 1176, 112742.	1.1	4
1104	Mechanism of Ir-catalyzed hydrogenation: A theoretical view. Coordination Chemistry Reviews, 2020, 412, 213251.	9.5	33
1105	Mechanistic Study on Gold-Catalyzed Cycloisomerization of Dienediynes Involving Aliphatic Câ€“H Functionalization and Inspiration for Developing a New Strategy to Access Polycarbocycles. Journal of the American Chemical Society, 2020, 142, 2777-2786.	6.6	42
1106	Ionization energies in solution with the QM:QM approach. Physical Chemistry Chemical Physics, 2020, 22, 10550-10560.	1.3	17
1107	A new database and benchmark of the bond energies of <scp>nobleâ€gas</scp>â€containing molecules. International Journal of Quantum Chemistry, 2020, 120, e26238.	1.0	6
1108	Reactivity of Î±,Ï‰-Dihydrofluoropolyethers toward OH Predicted by Multiconformer Transition State Theory and the Interacting Quantum Atoms Approach. Journal of Physical Chemistry A, 2020, 124, 3460-3470.	1.1	7
1109	Improving photosensitivity without changing thermal reactivity in photochromic diarylbenzenes based on accurate prediction by DFT calculations. Photochemical and Photobiological Sciences, 2020, 19, 644-653.	1.6	8

#	Article	IF	Citations
1110	Quantification of the mixed-valence and intervalence charge transfer properties of a cofacial metalâ€“organic framework via single crystal electronic absorption spectroscopy. Chemical Science, 2020, 11, 5213-5220.	3.7	18
1111	How accurate are TDâ€DFT excitedâ€state geometries compared to DFT groundâ€state geometries?. Journal of Computational Chemistry, 2020, 41, 1718-1729.	1.5	57
1112	On the Spectroscopic Modeling of Localized Defects in Sodalites by TD-DFT. Journal of Physical Chemistry C, 2020, 124, 8949-8957.	1.5	15
1113	The electronic states and vibronic absorption spectrum of berberine in aqueous solution. International Journal of Quantum Chemistry, 2021, 121, e26537.	1.0	5
1114	Pyridine-substituted triazine as an acceptor for thermally activated delayed fluorescence emitters showing high efficiency and low roll-off in organic light-emitting diodes. Materials Today Energy, 2021, 20, 100581.	2.5	6
1115	Photophysical Properties of Fluorescent 2â€(Phenylamino)â€1,10â€phenanthroline Derivatives â€. Photochemistry and Photobiology, 2021, 97, 47-60.	1.3	4
1116	Fitting elephants in the density functionals zoo: Statistical criteria for the evaluation of density functional theory methods as a suitable replacement for counting parameters. International Journal of Quantum Chemistry, 2021, 121, e26379.	1.0	7
1117	Self-consistent electrostatic embedding for liquid phase polarization. Journal of Molecular Liquids, 2021, 322, 114550.	2.3	7
1118	Hydrogen abstraction of alkyl radicals from polycyclic aromatic hydrocarbons and heterocyclic aromatic hydrocarbons. Chemical Engineering Science, 2021, 232, 116342.	1.9	7
1119	Monitoring peptide tyrosine nitration by spectroscopic methods. Amino Acids, 2021, 53, 517-532.	1.2	14
1120	A theoretical study of the potential energy surface for the isomerization reaction of fluoranthene to aceanthrylene: Implications for combustion chemistry. Computational and Theoretical Chemistry, 2021, 1196, 113118.	1.1	1
1121	Structures, energetics, and kinetics of H-atom abstraction from methyl propionate by molecular oxygen: Ab initio and DFT investigations. Computational and Theoretical Chemistry, 2021, 1196, 113119.	1.1	15
1122	The vibronic absorption spectra and electronic states of acridine orange in aqueous solution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 249, 119302.	2.0	5
1123	Superiority of Iridium Photocatalyst and Role of Quinuclidine in Selective Î±-C(sp³)â€“H Alkylation: Theoretical Insights. Journal of Organic Chemistry, 2021, 86, 484-492.	1.7	3
1124	Comprehensive Benchmark Study on the Calculation of ²⁹Si NMR Chemical Shifts. Inorganic Chemistry, 2021, 60, 272-285.	1.9	14
1125	Can density functional theory â€˜Copeâ€™ with highly fluxional shapeshifting molecules?. Chemical Physics, 2021, 540, 111013.	0.9	15
1126	Theoretical investigation of aromaticity and charge transfer in emission process of triarylmethyl radicals as <scp>OLED</scp> materials. International Journal of Quantum Chemistry, 2021, 121, e26522.	1.0	6
1127	Effect of substitution on dissociation kinetics of C₂H₅X, (Xâ€‰=â€‰F, Cl, Br and I): A theoretical study. Molecular Physics, 2021, 119, e1807635.	0.8	1

#	Article	IF	Citations
1128	Temperature evolution in IR action spectroscopy experiments with sodium doped water clusters. Physical Chemistry Chemical Physics, 2021, 23, 7682-7695.	1.3	7
1129	Structural characterisation of natural products by means of quantum chemical calculations of NMR parameters: new insights. Organic Chemistry Frontiers, 2021, 8, 2019-2058.	2.3	45
1130	Failure of molecular dynamics to provide appropriate structures for quantum mechanical description of the aqueous chloride ion charge-transfer-to-solvent ultraviolet spectrum. Physical Chemistry Chemical Physics, 2021, 23, 9109-9120.	1.3	1
1131	Multiple â€œHot excitonâ€•channel molecular design in organic electroluminescence materials: a theoretical investigation. Materials Advances, 2021, 2, 1351-1357.	2.6	12
1132	Replacing hybrid density functional theory: motivation and recent advances. Chemical Society Reviews, 2021, 50, 8470-8495.	18.7	80
1133	Fluxionality by quantum tunnelling: nonclassical 21-homododecahedryl cation rearrangement re-revisited. Chemical Communications, 2021, 57, 10735-10738.	2.2	1
1134	Predicting the structure and NMR coupling constant ¹J(¹²⁹Xeâ€“¹⁹F) of XeF₆ using quantum mechanics methods. Physical Chemistry Chemical Physics, 2021, 23, 7240-7246.	1.3	2
1135	The Vibronic Absorption Spectrum and Electronic States of Nile Red in Aqueous Solution. ChemistrySelect, 2021, 6, 1297-1304.	0.7	1
1136	What Types of Chemical Problems Benefit from Density-Corrected DFT? A Probe Using an Extensive and Chemically Diverse Test Suite. Journal of Chemical Theory and Computation, 2021, 17, 1368-1379.	2.3	45
1137	Quantitative characterisation of the ring normal modes. Pyridine as a study case. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 246, 119026.	2.0	11
1139	Methine-Quinoidal Fragment Induces Significant Bathochromic Shifts in Organic Dyes. Journal of Physical Chemistry B, 2021, 125, 1447-1452.	1.2	5
1140	Do Secondary Electrostatic Interactions Influence Multiple Dihydrogen Bonds? AAâ''DD Array on an Amineâ€Borane Azaâ€Coronand: Theoretical Studies and Synthesis. ChemPhysChem, 2021, 22, 593-605.	1.0	9
1141	The Devilâ€™s Triangle of Kohnâ€“Sham density functional theory and excited states. Journal of Chemical Physics, 2021, 154, 074106.	1.2	9
1142	The vibronic absorption spectra and electronic states of acridine yellow in aqueous solution. Journal of Molecular Liquids, 2021, 326, 115312.	2.3	7
1143	Accurate Prediction of MÃ¶ssbauer Hyperfine Parameters in Bis-Axially Coordinated Iron(II) Phthalocyanines Using Density Functional Theory Calculations: A Story of a Single Orbital Revealed by Natural Bond Orbital Analysis. Inorganic Chemistry, 2021, 60, 3690-3706.	1.9	13
1144	Ab initio-based kinetics of hydrogen atom abstraction from methyl propionate by H and CH3 radicals: a biodiesel model. Structural Chemistry, 2021, 32, 1857-1872.	1.0	12
1145	Packing Effect on Light Emission of Naphthyridine-Based Luminophor: Insights from Quantum Mechanics and Quantum Mechanics/Molecular Mechanics Calculations. Journal of Physical Chemistry B, 2021, 125, 3005-3013.	1.2	2
1146	Glycerol as a Substrate and Inactivator of Coenzyme B₁₂â€Dependent Diol Dehydratase. Chemistry - A European Journal, 2021, 27, 7930-7941.	1.7	4

#	Article	IF	Citations
1147	Computational Studies on Reactions of Some Organic Azides with Câ^'H Bonds. ChemistrySelect, 2021, 6, 4368-4381.	0.7	2
1148	Theoretical prediction of an NXeH4+ ion with N-Xe triple bond. Computational and Theoretical Chemistry, 2021, 1199, 113193.	1.1	2
1149	Theoretical study of the kinetics of F-atom abstraction reactions from F2, CF2(OF)2, CF3OF and SF5OF by CO. Molecular Physics, 0, , e1939899.	0.8	0
1150	Mixedâ€Valence Compounds as Polarizing Agents for Overhauser Dynamic Nuclear Polarization in Solids**. Angewandte Chemie - International Edition, 2021, 60, 15371-15375.	7.2	18
1151	Evaluation of density functional theory for a large and diverse set of organic and inorganic equilibrium structures. Journal of Computational Chemistry, 2021, 42, 1590-1601.	1.5	44
1152	Gemischtvalente Verbindungen als polarisierende Mittel fÃ¼r die dynamische Kernâ€Overhauserâ€Polarisation in FestkÃ¶rpern**. Angewandte Chemie, 2021, 133, 15499-15503.	1.6	0
1153	Photochemistry of Nâ€Phenyl Dibenzothiophene Sulfoximine^{â€}. Photochemistry and Photobiology, 2021, 97, 1322-1334.	1.3	11
1154	Thermochemical and kinetic studies of hydrogen abstraction reaction from C16H10 isomers by H atoms. Computational and Theoretical Chemistry, 2021, 1201, 113257.	1.1	4
1155	First-principle kinetic studies of unimolecular pyrolysis of isopropyl esters as biodiesel surrogates. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	8
1156	A DFT study on OH radical scavenging activities of eriodictyol, Isosakuranetin and pinocembrin. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10802-10811.	2.0	6
1157	Density Functional Geometries and Zero-Point Energies in Ab Initio Thermochemical Treatments of Compounds with First-Row Atoms (H, C, N, O, F). Journal of Chemical Theory and Computation, 2021, 17, 4872-4890.	2.3	22
1158	Benchmarking of Density Functionals for Z-Azoarene Half-Lives via Automated Transition State Search. Journal of Physical Chemistry A, 2021, 125, 6474-6485.	1.1	8
1159	OH-initiated degradation of methyl 2-chloroacetoacetate and ethyl 2-chloroacetoacetate: Kinetics, products and mechanisms at 298ÂK and atmospheric pressure. Chemosphere, 2021, 274, 129659.	4.2	2
1160	Density Functional Theory for Electrocatalysis. Energy and Environmental Materials, 2022, 5, 157-185.	7.3	95
1161	Assessment of the Accuracy of DFT-Predicted Li⁺â€“Nucleic Acid Binding Energies. Journal of Chemical Theory and Computation, 2021, 17, 5392-5408.	2.3	4
1162	Theoretical study on pentiptycene molecular brake: photoinduced isomerization and photoinduced electron transfer. Journal of Molecular Modeling, 2021, 27, 289.	0.8	0
1163	Low-Order Scaling Quasiparticle Self-Consistent GW for Molecules. Frontiers in Chemistry, 2021, 9, 736591.	1.8	24
1164	Dual-channel D-(Ï€-A)2 phenoxazine/phenothiazine dyes with an auxiliary N-alkoxy benzoic acid anchor for fabrication of dye-sensitized solar cells. Solar Energy, 2021, 225, 173-183.	2.9	9

#	Article	IF	Citations
1165	Theoretical design study on the origin of the improved phosphorescent efficiency of DPEphos quinoline-substituted derivatives for OLEDs. Organic Electronics, 2021, 97, 106185.	1.4	1
1166	Low-temperature oxidation of monobromobenzene: Bromine transformation and yields of phenolic species. Chemosphere, 2021, 280, 130621.	4.2	8
1167	Shapeshifting radicals. Chemical Physics, 2022, 552, 111373.	0.9	1
1168	Unknown Knowns: Case studies in uncertainties in the computation of thermochemical parameters. Chemical Physics, 2021, 550, 111251.	0.9	0
1169	Assessment of density functional theory in studying on the transition states of a Diiron-mediated N N bond cleavage reaction. Computational and Theoretical Chemistry, 2021, 1204, 113418.	1.1	1
1170	Adsorption properties of two-dimensional carbon material towards the heavy metal ions. Journal of Molecular Liquids, 2021, 342, 117500.	2.3	4
1171	Biodiesel combustion: Kinetics and thermochemistry of H-atom abstraction from methyl propionate by Ã– (3P) and O2H radicals: ab initio study. Journal of Molecular Structure, 2021, 1243, 130896.	1.8	0
1172	Temperature-dependent profiles of dioxin-like toxicants from combustion of brominated flame retardants. Journal of Hazardous Materials, 2022, 422, 126879.	6.5	17
1173	Hydride Affinities for Main-Group Hydride Reductants: Assessment of Density Functionals and Trends in Reactivities. Journal of Physical Chemistry A, 2021, 125, 835-842.	1.1	7
1174	Mechanism investigation on the reaction of methylmethoxy radical with nitrogen monoxide. Structural Chemistry, 2021, 32, 1563-1570.	1.0	0
1175	Impact of fluorination and chlorination on the electronic structure, topology and in-plane ring normal modes of pyridines. Physical Chemistry Chemical Physics, 2021, 23, 18958-18974.	1.3	5
1176	Substituent effects on through-space intervalence charge transfer in cofacial metalâ€“organic frameworks. Faraday Discussions, 2021, 231, 152-167.	1.6	2
1177	Theoretical study on adiabatic electron affinity of fatty acids. New Journal of Chemistry, 2021, 45, 16892-16905.	1.4	4
1178	Efficient and organic hostâ€“guest room-temperature phosphorescence: tunable tripletâ€“singlet crossing and theoretical calculations for molecular packing. Chemical Science, 2021, 12, 6518-6525.	3.7	83
1179	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
1180	Exchange-Correlation Functionals. , 2014, , 101-124.		1
1181	Computational Perspectives on Organolithium Carbenoids. , 2012, , 471-510.		4
1182	Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response. Journal of Chemical Physics, 2020, 152, 044111.	1.2	22

#	Article	IF	Citations
1183	Unveiling the role of short-range exact-like exchange in the optimally tuned range-separated hybrids for fluorescence lifetime modeling. Journal of Chemical Physics, 2020, 152, 204301.	1.2	8
1184	Performance of Density Functionals for the Calculation of Gold Clusters. Bulletin of the Korean Chemical Society, 2011, 32, 2802-2804.	1.0	5
1185	Aggregation effects on photophysical properties of NBN-doped polycyclic aromatic hydrocarbons: a theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 23986-23997.	1.3	10
1186	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
1187	The Reactive Sites of Methane Activation: A Comparison of IrC3+ with PtC3+. Molecules, 2021, 26, 6028.	1.7	3
1188	Performance of new exchangeâ€“correlation functionals in providing vertical excitation energies of metal complexes. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	3
1189	Theoretical analysis of lactone and carboxylate forms of camptothecin in aqueous solution: Electronic states, absorption spectra, and hydration. Journal of Molecular Liquids, 2021, 344, 117804.	2.3	8
1190	Generalized gradient exchange functionals based on the gradient-regulated connection: a new member of the TCA family. Highlights in Theoretical Chemistry, 2013, , 237-243.	0.0	0
1191	Density functional theory for the description of charge-transfer processes at TTF/TCNQ interfaces. Highlights in Theoretical Chemistry, 2014, , 217-224.	0.0	0
1192	Density functional and chemical model study of the competition between methyl and hydrogen scission of propane and Î²-scission of the propyl radical. Highlights in Theoretical Chemistry, 2014, , 63-80.	0.0	0
1193	A simple DFT-based diagnostic for nondynamical correlation. Highlights in Theoretical Chemistry, 2014, , 251-259.	0.0	0
1194	An Overview of Modern Density Functional Theory. Springer Briefs in Molecular Science, 2014, , 1-24.	0.1	0
1195	Density Functional Theory. Encyclopedia of Earth Sciences Series, 2018, , 347-352.	0.1	0
1198	Platinum(II) Complexes of Tridentate â€Coordinating Ligands Based on Imides, Amides, and Hydrazides: Synthesis and Luminescence Properties. European Journal of Inorganic Chemistry, 2021, 2021, 335-347.	1.0	9
1199	The synthesis of pyrrole from C4â€olefinated isoxazole catalyzed by ruthenium: A density functional theory study. Journal of Physical Organic Chemistry, 2021, 34, e4178.	0.9	2
1200	Thermally activated delayed fluorescence materials with aggregation-induced emission properties: a QM/MM study. Physical Chemistry Chemical Physics, 2021, 23, 25789-25796.	1.3	10
1201	Aggregation-induced emission spectra of triphenylamine salicylaldehyde derivatives via excited-state intramolecular proton transfer revealed by molecular spectral and dynamics simulations. RSC Advances, 2021, 11, 37171-37180.	1.7	5
1202	Unveiling the mechanisms of organic room-temperature phosphorescence in various surrounding environments: a computational study. Physical Chemistry Chemical Physics, 2021, 23, 26813-26821.	1.3	6

#	Article	IF	Citations
1203	An inexpensive density functional theory â€b based protocol to predict accurate 19 Fâ€NMR chemical shifts. Journal of Computational Chemistry, 2022, 43, 170-183.	1.5	5
1204	Glycolonitrile (HOCH₂CN) Chemistry in Star-forming Regions. Astrophysical Journal, Supplement Series, 2021, 257, 26.	3.0	4
1205	Degradation mechanism of 2-fluoropropene by Cl atoms: experimental and theoretical products distribution studies. Physical Chemistry Chemical Physics, 2022, , .	1.3	1
1206	A two-step MM and QM/MM approach to model AIEE of aryloxy benzothiadiazole derivatives for optoelectronic applications. Physical Chemistry Chemical Physics, 2022, 24, 4051-4064.	1.3	6
1207	Catalytic upgrading of the polymeric constituents in Covid-19 masks. Journal of Environmental Chemical Engineering, 2022, 10, 106978.	3.3	23
1208	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
1209	Theoretically elucidating high photoluminescence performance of dimethylacridan-based blue-color thermally activated delayed fluorescent materials. New Journal of Chemistry, 2022, 46, 3464-3471.	1.4	7
1210	Not the sum of their parts: understanding multi-donor interactions in symmetric and asymmetric TADF emitters. Journal of Materials Chemistry C, 2022, 10, 4737-4747.	2.7	11
1211	Structureâ€“property relationship study of blue thermally activated delayed fluorescence molecules with different donor and position substitutions: theoretical perspective and molecular design. Journal of Materials Chemistry C, 2022, 10, 4723-4736.	2.7	17
1212	The MOBH35 Metalâ€“Organic Barrier Heights Reconsidered: Performance of Local-Orbital Coupled Cluster Approaches in Different Static Correlation Regimes. Journal of Chemical Theory and Computation, 2022, 18, 883-898.	2.3	27
1213	Towards Elucidating Structureâ€“Spectra Relationships in Rhamnogalacturonan II: Computational Protocols for Accurate 13C and 1H Shifts for Apiose and Its Borate Esters. Frontiers in Molecular Biosciences, 2021, 8, 756219.	1.6	0
1214	Free Energy Profiles of Proton Transfer Reactions: Density Functional Benchmark from Biased Ab Initio Dynamics. Journal of Chemical Theory and Computation, 2022, , .	2.3	5
1215	Accurate redox potentials for solvents in <scp>Liâ€metal</scp> batteries and assessment of density functionals. International Journal of Quantum Chemistry, 2022, 122, .	1.0	6
1216	Mechanism and Stereochemistry of Rhodium-Catalyzed [5 + 2 + 1] Cycloaddition of Eneâ€“Vinylcyclopropanes and Carbon Monoxide Revealed by Visual Kinetic Analysis and Quantum Chemical Calculations. Journal of the American Chemical Society, 2022, 144, 2624-2636.	6.6	21
1217	Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585.		0
1218	A theoretical study on the proton affinity of sulfur ylides. New Journal of Chemistry, 0, , .	1.4	5
1219	The duhka of DFT: a noble path to better functionals via a point electron approximation for the exchangeâ€“correlation hole â€ , â€¡. Australian Journal of Chemistry, 2022, , .	0.5	2
1220	A framework for scintillation in nanophotonics. Science, 2022, 375, eabm9293.	6.0	59

#	Article	IF	Citations
1221	Generalized energy-based fragmentation approach for accurate binding energies and Raman spectra of methane hydrate clusters. Chinese Journal of Chemical Physics, 2022, 35, 167-176.	0.6	3
1222	Determining the Energy Gap between the S₁ and T₁ States of Thermally Activated Delayed Fluorescence Molecular Systems Using Transient Fluorescence Spectroscopy. Journal of Physical Chemistry Letters, 2022, 13, 2507-2515.	2.1	12
1223	Ca2C MXene monolayer as a superior material for detection of toxic pnictogen hydrides. Materials Chemistry and Physics, 2022, 281, 125869.	2.0	4
1224	Experimental and theoretical study of organic sensitizers for solid-state dye-sensitized solar cells (s-DSSCs). Journal of Photochemistry and Photobiology A: Chemistry, 2022, 428, 113890.	2.0	6
1225	Attochemistry of hydrogen bonded amide and thioamide model complexes in protein following vertical ionization. Chemical Physics, 2022, 559, 111508.	0.9	1
1226	Electronic Energy and Local Property Errors at QTAIM Critical Points while Climbing Perdewâ€™s Ladder of Density-Functional Approximations. Journal of Chemical Theory and Computation, 2022, 18, 293-308.	2.3	14
1227	Benchmarking Density Functional Approximations for Excited-State Properties of Fluorescent Dyes. Molecules, 2021, 26, 7434.	1.7	13
1228	Odd-Number Cyclo[n]Carbons Sustaining Alternating Aromaticity. Journal of Physical Chemistry A, 2022, 126, 2445-2452.	1.1	7
1233	Gliding on Ice in Search of Accurate and Cost-Effective Computational Methods for Astrochemistry on Grains: The Puzzling Case of the HCN Isomerization. Journal of Chemical Theory and Computation, 2022, 18, 3111-3121.	2.3	4
1234	Charge transfer in mixed and segregated stacks of tetrathiafulvalene, tetrathianaphthalene and naphthalene diimide: a structural, spectroscopic and computational study. New Journal of Chemistry, 0, , .	1.4	0
1235	A quantum chemistry study on Câ€“H homolytic bond dissociation enthalpies of five-membered and six-membered heterocyclic compounds. Journal of the Indian Chemical Society, 2022, 99, 100527.	1.3	1
1236	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. Physica Scripta, 2022, 97, 065808.	1.2	7
1237	Revisiting the Performance of Time-Dependent Density Functional Theory for Electronic Excitations: Assessment of 43 Popular and Recently Developed Functionals from Rungs One to Four. Journal of Chemical Theory and Computation, 2022, 18, 3460-3473.	2.3	61
1238	Charge-Transfer Spectroscopy of Bisaxially Coordinated Iron(II) Phthalocyanines through the Prism of the Leverâ€™s E_L Parameters Scale, MCD Spectroscopy, and TDDFT Calculations. Inorganic Chemistry, 2022, 61, 8250-8266.	1.9	6
1239	Insights on isomeric emitters with thermally activated delayed fluorescence: Comparison between solvent and crystal state. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 278, 121328.	2.0	4
1240	A mechanistic view of the reaction between phosphine and fluorine atom: Insights into PH3F isomers. Computational and Theoretical Chemistry, 2022, 1214, 113769.	1.1	0
1242	Efficient and Accurate Description of Dielsâ€Alder Reactions Using Density Functional Theory**. ChemPhysChem, 2022, 23, .	1.0	6
1243	Reaction of Ta₃^{â€“} Clusters with Molecular Nitrogen: A Mechanism Investigation. ACS Omega, 2022, 7, 22682-22688.	1.6	3

#	Article	IF	Citations
1244	Niobium and Tantalum Octahedral Halides: Vibrational Properties and Intraâ€“Cluster Interactions. SSRN Electronic Journal, 0, , .	0.4	0
1245	Impact of the current density on paramagnetic NMR properties. Journal of Chemical Physics, 2022, 157, .	1.2	13
1246	Thermallyâ€Activated Tunneling in the Twoâ€Water Bridge Catalyzed Tautomerization of Phosphinylidene Compounds**. ChemPhysChem, 2022, 23, .	1.0	1
1247	Why [4 + 2 + 1] but Not [2 + 2 + 1]? Why Allenes? A Mechanistic Study of the Rhodium-Catalyzed [4 + 2 + 1] Cycloaddition of In Situ Generated Eneâ€“Eneâ€“Allenes and Carbon Monoxide. Journal of Organic Chemistry, 2022, 87, 10576-10591.	1.7	3
1248	Benefits of Range-Separated Hybrid and Double-Hybrid Functionals for a Large and Diverse Data Set of Reaction Energies and Barrier Heights. Journal of Physical Chemistry A, 2022, 126, 5492-5505.	1.1	11
1249	Theoretical study of the Meisenheimer and charge-transfer complexes formed upon colorimetric determination of nitroaromatic explosives. FirePhysChem, 2022, , .	1.5	1
1250	Study on the activation mechanism of protactinium and NH3 by density functional theory. Chemical Physics Letters, 2022, 806, 140072.	1.2	0
1251	Tuning ESIPT-coupled luminescence by expanding Ï€-conjugation of a proton acceptor moiety in ESIPT-capable zinc(<scp>ii</scp>) complexes with 1-hydroxy-1H-imidazole-based ligands. Dalton Transactions, 2022, 51, 15166-15188.	1.6	11
1252	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
1253	Suppression of reversible photocyclization reaction induced fluorescence enhancement: a theoretical study. Physical Chemistry Chemical Physics, 2022, 24, 25487-25494.	1.3	5
1254	Rational designs of structurally similar TADF and HLCT emitters with benzo- or naphtho-carbazole units as electron donors. Physical Chemistry Chemical Physics, 0, , .	1.3	1
1255	Insight into through-space conjugation in rotation-restricted thermally activated delayed fluorescence compounds. Journal of Materials Chemistry C, 2022, 10, 15152-15159.	2.7	3
1256	Octa-coordination in complexes of lanthanides with N2 confirmed by matrix-isolation IR spectroscopy and DFT calculations. Journal of Molecular Structure, 2023, 1272, 134222.	1.8	3
1257	Predicting and Designing Thermally Activated Delayed Fluorescence Molecules with Balanced Î”E_{ST} and Transition Dipole Moment. Advanced Theory and Simulations, 2022, 5, .	1.3	5
1258	The performance of exchangeâ€”correlation functionals in describing electron density parameters of saddle point structures along chemical reactions. Journal of Computational Chemistry, 2022, 43, 1830-1838.	1.5	1
1259	A DFT Study on the Excited Electronic States of Cyanopolyynes: Benchmarks and Applications. Molecules, 2022, 27, 5829.	1.7	3
1260	Importance of imposing gauge invariance in time-dependent density functional theory calculations with meta-generalized gradient approximations. Journal of Chemical Physics, 2022, 157, .	1.2	7
1261	Bestâ€Practice DFT Protocols for Basic Molecular Computational Chemistry**. Angewandte Chemie, 2022, 134, .	1.6	36

#	Article	IF	Citations
1262	Bestâ€Practice DFT Protocols for Basic Molecular Computational Chemistry**. Angewandte Chemie - International Edition, 2022, 61, .	7.2	168
1263	Revisiting fundamental properties of TiO₂ nanoclusters as condensation seeds in astrophysical environments. Astronomy and Astrophysics, 2022, 668, A35.	2.1	5
1264	Electronic band structure of Bi5O7NO3 and its methyl orange removal mechanism. European Journal of Chemistry, 2022, 13, 337-350.	0.3	0
1265	Efficient deep red/near-infrared thermally activated delayed fluorescence emitters via molecular reconstruction: theoretical insights. Physical Chemistry Chemical Physics, 2022, 24, 26764-26775.	1.3	4
1266	Accurate Nonempirical Range-Separated Hybrid van der Waals Density Functional for Complex Molecular Problems, Solids, and Surfaces. Physical Review X, 2022, 12, .	2.8	5
1267	A Theoretical Investigation into the Homo- and Hetero-leptic Cu(I) Phosphorescent Complexes Bearing 2,9-dimethyl-1,10-phenanthroline and bis [2-(diphenylphosphino)phenyl]ether Ligand. Materials, 2022, 15, 7253.	1.3	1
1268	Endowing homodimeric carbamoyltransferase GdmN with iterative functions through structural characterization and mechanistic studies. Nature Communications, 2022, 13, .	5.8	1
1269	Dual Activation Strategy to Achieve Câ€“C Cleavage of Cyclobutanes: Development and Mechanism of Rh and Zn Cocatalyzed [4 + 2] Cycloaddition of Yne-Vinylcyclobutanones. Journal of the American Chemical Society, 2022, 144, 21457-21469.	6.6	6
1270	Insights into glycosidic bond specificity of an engineered selective Î±-L-rhamnosidase N12-Rha via activity assays and molecular modelling. AMB Express, 2022, 12, .	1.4	2
1271	Investigation of G4(MP2)-XK theory for antimony compoundsâ€™ thermochemistry. Journal of Molecular Modeling, 2022, 28, .	0.8	2
1272	High-level quantum chemistry exploration of reduction by group-13 hydrides: insights into the rational design of bio-mimic CO₂ reduction. Electronic Structure, 2022, 4, 044001.	1.0	0
1273	A comprehensive benchmark investigation of quantum chemical methods for carbocations. Physical Chemistry Chemical Physics, 2023, 25, 1903-1922.	1.3	3
1274	Bond dissociation energies of Xâ€“H bonds in proteins. RSC Advances, 2022, 12, 34557-34564.	1.7	4
1275	Resolving a Half-Century-Long Controversy between (Magneto)optical and EPR Spectra of Single-Electron-Reduced [PcFe]^{â^'}, [PcFeL]^{â^'}, and [PcFeX]^{2â€“} Complexes: Story of a Double Flip. Inorganic Chemistry, 2022, 61, 20177-20199.	1.9	3
1276	Molecular docking and A DFT study on the antiradical activity of naringenin and hesperetin with nitric oxide, peroxy, and methoxy radicals. Journal of Physical Organic Chemistry, 0, , .	0.9	0
1277	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
1278	TDDFT versus GW/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
1279	Interexcited State Photophysics I: Benchmarking Density Functionals for Computing Nonadiabatic Couplings and Internal Conversion Rate Constants. Journal of Chemical Theory and Computation, 2023, 19, 271-292.	2.3	5

#	Article	IF	Citations
1280	Theoretical Study on Non-Linear Optics Properties of Polycyclic Aromatic Hydrocarbons and the Effect of Their Intercalation with Carbon Nanotubes. Molecules, 2023, 28, 110.	1.7	1
1281	Metallaâ€Claisen Rearrangement in Goldâ€Catalyzed [4 + 2] Reaction: A New Elementary Reaction Suggested for Future Reaction Design. Angewandte Chemie - International Edition, 0, , .	7.2	2
1282	Atomistic insight into the effects of electrostatic fields on hydrocarbon reaction kinetics. Journal of Chemical Physics, 2023, 158, .	1.2	1
1283	Stereoselective Synthesis and Biological Profile of All Stereoisomers of Lactam Analogues of Strigolactones GR24 and GR18. Helvetica Chimica Acta, 2023, 106, .	1.0	0
1284	Metallaâ€Claisen Rearrangement in Goldâ€Catalyzed [4 + 2] Reaction: A New Elementary Reaction Suggested for Future Reaction Design. Angewandte Chemie, 0, , .	1.6	0
1286	The Highly Exothermic Hydrogen Abstraction Reaction H2Te + OH â†' H2O + TeH: Comparison with Analogous Reactions for H2Se and H2S. Physical Chemistry Chemical Physics, 0, , .	1.3	0
1287	Effect of Aggregation on Thermally Activated Delayed Fluorescence and Ultralong Organic Phosphorescence: QM/MM Study. Chinese Physics B, 0, , .	0.7	0
1288	Thymus satureoides Oil as Green Corrosion Inhibitor for 316L Stainless Steel in 3% NaCl: Experimental and Theoretical Studies. Lubricants, 2023, 11, 56.	1.2	6
1290	Theoretical study of the excitation of proflavine H-dimers in an aqueous solution: the effect of functionals and dispersion corrections. Physical Chemistry Chemical Physics, 2023, 25, 12259-12276.	1.3	4
1291	Carbonyl (Cî€O)/N-based thermally activated delayed fluorescent materials with high efficiency and fast reverse intersystem crossing rate: a theoretical design and study. New Journal of Chemistry, 2023, 47, 7686-7693.	1.4	2
1292	Graphene Catalysis Made Easy. , 2024, , 580-593.		0
1293	Theoretical study on the mechanism of aggregation-induced emission in red thermally activated delayed fluorescence molecules: trans/cis-arrangement effect. Organic Electronics, 2023, 119, 106811.	1.4	0
1294	Pyrolytic elimination of ethylene from ethoxyquinolines and ethoxyisoquinolines: a computational study. Scientific Reports, 2023, 13, .	1.6	3
1295	Characterizing excited states of single donor-acceptor molecule by high-resolution Raman images. Physics Letters, Section A: General, Atomic and Solid State Physics, 2023, 461, 128648.	0.9	1
1296	Computational Study of Mechanisms and Tether Length Effects of Rhâ€Catalyzed [3+2] and [3+2+1] Reactions of Ene/Yneâ€Vinylcyclopropanes. Chemistry - an Asian Journal, 2023, 18, .	1.7	0
1297	Improving the TADF in Corannuleneâ€Based Emitters via Tuning the Strength of Donor and Acceptor Groups. Advanced Theory and Simulations, 2023, 6, .	1.3	0
1298	Unprecedented endo-oxidative cyclometallation and [4Â+ 3] cycloaddition of diene-vinylcyclopropanes. CheM, 2023, 9, 1477-1494.	5.8	3
1299	Strain-Release-Controlled [4 + 2 + 1] Reaction of Cyclopropyl-Capped Diene-ynes/Diene-enes and Carbon Monoxide Catalyzed by Rhodium. Journal of the American Chemical Society, 2023, 145, 5496-5505.	6.6	7

#	Article	IF	Citations
1300	How Doping Affects the Activity of the Aluminum Oxide Support. ChemPhysChem, 2023, 24, .	1.0	0
1301	Theoretical insights into luminescence mechanism of Naphthyridine-based thermally activated delayed fluorescence emitter with aggregation-induced emission. Chemical Physics Letters, 2023, 817, 140407.	1.2	3
1302	Influence of alkyl chain length on the photovoltaic properties of dithienopyran-based hole-transporting materials for perovskite solar cells. Journal of Materials Chemistry C, 2023, 11, 8223-8230.	2.7	1
1303	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
1304	Carbon Dioxide and Water Activation by Niobium Trioxide Anions in the Gas Phase. Journal of Physical Chemistry A, 2023, 127, 3402-3411.	1.1	1
1305	Comparison of the Performance of Density Functional Methods for the Description of Spin States and Binding Energies of Porphyrins. Molecules, 2023, 28, 3487.	1.7	3
1306	Thermochemistry of the Smallest Hyperbolic Paraboloid Hydrocarbon: A High-Level Quantum Chemical Perspective. Journal of Carbon Research, 2023, 9, 41.	1.4	0
1312	Electron-density-based analysis and electron density functional theory (DFT) methods. , 2023, , 177-197.		0
1318	Density-functional theory for electronic excited states. , 2023, , 69-118.		7
1341	Simulating excited states in metal organic frameworks: from light-absorption to photochemical CO₂ reduction. Materials Advances, 0, , .	2.6	0
1346	Computer-assisted Study of Garlic Organosulfur as Antioxidant Agents. , 2023, , 62-82.		0