

Efficient and Accurate Double-Hybrid-Meta-GGA Densities
Extended GMTKN30 Database for General Main Group
Noncovalent Interactions

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Citation Report

#	ARTICLE	IF	CITATIONS
12	Titanium Oxide Complexes with Dinitrogen. Formation and Characterization of the Side-On and End-On Bonded Titanium Oxide–Dinitrogen Complexes in Solid Neon. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6551-6558.	2.5	20
13	Ab Initio Modeling of Donor–Acceptor Interactions and Charge-Transfer Excitations in Molecular Complexes: The Case of Terthiophene–Tetracyanoquinodimethane. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2068-2077.	5.3	46
14	Formation of N–N Cross-Links in DNA by Reaction of Radiation-Produced DNA Base Pair Diradicals: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 15090-15097.	2.6	11
15	Accuracy of Density Functionals in the Prediction of Electronic Proton Affinities of Amino Acid Side Chains. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3898-3908.	5.3	45
16	Benchmarking Semiempirical Methods for Thermochemistry, Kinetics, and Noncovalent Interactions: OMx Methods Are Almost As Accurate and Robust As DFT-GGA Methods for Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2929-2936.	5.3	89
17	A Parameter-Free Density Functional That Works for Noncovalent Interactions. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 983-989.	4.6	134
18	Accurate Dispersion-Corrected Density Functionals for General Chemistry Applications. , 2011, , 1-16.		2
19	Accuracy of Calculated Chemical Shifts in Carbon 1s Ionization Energies from Single-Reference <i>ab Initio</i> Methods and Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4104-4114.	5.3	29
20	S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2427-2438.	5.3	821
21	Efficient and accurate local single reference correlation methods for high-spin open-shell molecules using pair natural orbitals. <i>Journal of Chemical Physics</i> , 2011, 135, 214102.	3.0	165
22	One Product, Two Pathways: Initially Divergent Radical Reactions Reconverge To Form a Single Product in High Yield. <i>Journal of the American Chemical Society</i> , 2011, 133, 16270-16276.	13.7	31
23	Two-Dimensional Scan of the Performance of Generalized Gradient Approximations with Perdew–Burke–Ernzerhof-Like Enhancement Factor. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3548-3559.	5.3	49
24	Density Functional Theory Studies of the Extent of Hole Delocalization in One-Electron Oxidized Adenine and Guanine Base Stacks. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4990-5000.	2.6	55
25	Accurate Interaction Energies for Problematic Dispersion-Bound Complexes: Homogeneous Dimers of NCCN, P2, and PCCP. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2842-2851.	5.3	46
26	Extensions of the S66 Data Set: More Accurate Interaction Energies and Angular-Displaced Nonequilibrium Geometries. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3466-3470.	5.3	201
27	Obtaining Good Performance With Triple- η -Type Basis Sets in Double-Hybrid Density Functional Theory Procedures. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2852-2863.	5.3	59
28	Assessment of Theoretical Methods for Complexes of Gold(I) and Gold(III) with Unsaturated Aliphatic Hydrocarbon: Which Density Functional Should We Choose?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4002-4011.	5.3	113
29	DSD-PBEP86: in search of the best double-hybrid DFT with spin-component scaled MP2 and dispersion corrections. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20104.	2.8	409

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30	Validation of electronic structure methods for isomerization reactions of large organic molecules. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13683.	2.8	78
31	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3567-3577.	5.3	400
32	Further evidences of the quality of double-hybrid energy functionals for π -conjugated systems. <i>Journal of Chemical Physics</i> , 2011, 134, 234102.	3.0	6
33	Performance of the van der Waals Density Functional VV10 and (hybrid)GGA Variants for Thermochemistry and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3866-3871.	5.3	213
34	Basis set convergence of explicitly correlated double-hybrid density functional theory calculations. <i>Journal of Chemical Physics</i> , 2011, 135, 144119.	3.0	29
35	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6670.	2.8	1,627
36	Electronic Control of Frustrated Lewis Pair Behavior: Chemistry of a Geminal Alkylidene-Bridged Per-pentafluorophenylated P/B Pair. <i>Organometallics</i> , 2011, 30, 4211-4219.	2.3	101
37	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3944-3951.	5.3	265
38	Density functional theory with London dispersion corrections. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 211-228.	14.6	2,030
39	Assessment of theoretical procedures for hydrogen-atom abstraction by chlorine, and related reactions. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 251-260.	1.4	37
40	On the Importance of the Dispersion Energy for the Thermodynamic Stability of Molecules. <i>ChemPhysChem</i> , 2011, 12, 1258-1261.	2.1	188
41	Oxidative Addition of the $C\equiv C$ Bond in α -O Linkage of Lignin to Transition Metals Using a Relativistic Pseudopotential-Based ccCA-ONIOM Method. <i>ChemPhysChem</i> , 2011, 12, 3320-3330.	2.1	26
42	System-Dependent Dispersion Coefficients for the DFT-D3 Treatment of Adsorption Processes on Ionic Surfaces. <i>ChemPhysChem</i> , 2011, 12, 3414-3420.	2.1	318
43	Benchmarking Density Functional Methods against the S66 and S66x8 Datasets for Non-Covalent Interactions. <i>ChemPhysChem</i> , 2011, 12, 3421-3433.	2.1	283
44	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. <i>Chemical Physics Letters</i> , 2011, 510, 165-178.	2.6	353
45	Density functional study of multiplicity-changing valence and Rydberg excitations of p-block elements: Delta self-consistent field, collinear spin-flip time-dependent density functional theory (DFT), and conventional time-dependent DFT. <i>Journal of Chemical Physics</i> , 2011, 135, 044118.	3.0	57
46	A systematic study of neutral and charged 3d-metal trioxides and tetraoxides. <i>Journal of Chemical Physics</i> , 2011, 134, 144305.	3.0	54
47	Long-range correlation energies from frequency-dependent weighted exchange-hole dipole polarisabilities. <i>Journal of Chemical Physics</i> , 2012, 136, 014104.	3.0	15

#	ARTICLE	IF	CITATIONS
48	B2-PPW91: A promising double-hybrid density functional for the electric response properties. Journal of Chemical Physics, 2012, 136, 124111.	3.0	30
49	The MP2 binding energy of the ethene dimer and its dependence on the auxiliary basis sets: a benchmark study using a newly developed infrastructure for the processing of quantum chemical data. Molecular Physics, 2012, 110, 2523-2534.	1.7	7
50	Strained and Unstrained Macrocycles Composed of Carbazole and Butadiyne Units: Electronic State and Optical Properties. Journal of Organic Chemistry, 2012, 77, 4837-4841.	3.2	10
51	Why the Standard B3LYP/6-31G* Model Chemistry Should Not Be Used in DFT Calculations of Molecular Thermochemistry: Understanding and Correcting the Problem. Journal of Organic Chemistry, 2012, 77, 10824-10834.	3.2	407
52	A geometrical correction for the inter- and intra-molecular basis set superposition error in Hartree-Fock and density functional theory calculations for large systems. Journal of Chemical Physics, 2012, 136, 154101.	3.0	556
53	JACOB: A Dynamic Database for Computational Chemistry Benchmarking. Journal of Chemical Information and Modeling, 2012, 52, 3255-3262.	5.4	4
54	Second-Order Møller-Plesset Perturbation Theory in the Condensed Phase: An Efficient and Massively Parallel Gaussian and Plane Waves Approach. Journal of Chemical Theory and Computation, 2012, 8, 4177-4188.	5.3	124
55	Metal-Free Aromatic Hydrogenation: Aniline to Cyclohexyl-amine Derivatives. Journal of the American Chemical Society, 2012, 134, 4088-4091.	13.7	154
57	Modeling Molecular Crystals by QM/MM: Self-Consistent Electrostatic Embedding for Geometry Optimizations and Molecular Property Calculations in the Solid. Journal of Chemical Theory and Computation, 2012, 8, 498-508.	5.3	39
58	Effects of Heterogeneity in Small π -Type Dimers: Homogeneous and Mixed Dimers of Diacetylene and Cyanogen. Journal of Chemical Theory and Computation, 2012, 8, 4279-4284.	5.3	5
59	BDE261: A Comprehensive Set of High-Level Theoretical Bond Dissociation Enthalpies. Journal of Physical Chemistry A, 2012, 116, 4975-4986.	2.5	62
60	Comparative Study of Single and Double Hybrid Density Functionals for the Prediction of 3d Transition Metal Thermochemistry. Journal of Chemical Theory and Computation, 2012, 8, 4102-4111.	5.3	69
61	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. Journal of Chemical Physics, 2012, 136, 174103.	3.0	99
62	Calculation of Host-Guest Binding Affinities Using a Quantum-Mechanical Energy Model. Journal of Chemical Theory and Computation, 2012, 8, 2023-2033.	5.3	60
63	Empirical Correction of Nondynamical Correlation Energy for Density Functionals. Journal of Physical Chemistry A, 2012, 116, 9969-9978.	2.5	16
64	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.	5.3	60
65	Thioformyl chloride dimer: An excellent model system for the assessment of new computational methods. Computational and Theoretical Chemistry, 2012, 983, 83-87.	2.5	2
66	Comparison of some dispersion-corrected and traditional functionals with CCSD(T) and MP2 ab initio methods: Dispersion, induction, and basis set superposition error. Journal of Chemical Physics, 2012, 137, 134109.	3.0	49

#	ARTICLE	IF	CITATIONS
67	Approaches for Obtaining Accurate Rate Constants for Hydrogen Abstraction by a Chlorine Atom. Journal of Physical Chemistry A, 2012, 116, 3745-3752.	2.5	29
68	XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. Physical Chemistry Chemical Physics, 2012, 14, 12554.	2.8	32
69	8.27 Spectroscopic Analysis: Ab initio Calculation of Chiroptical Spectra. , 2012, , 520-544.		4
70	A multiconfigurational hybrid density-functional theory. Journal of Chemical Physics, 2012, 137, 044104.	3.0	77
71	Comment on "Thioformyl chloride dimer: An excellent model system for the assessment of new computational methods" [Comput. Theoret. Chem. 983 (2012) 83-87]. Computational and Theoretical Chemistry, 2012, 999, 152-153.	2.5	0
72	Explicitly correlated W_{∞} theory: W1-F12 and W2-F12. Journal of Chemical Physics, 2012, 136, 124114.	3.0	229
73	Investigating inclusion complexes using quantum chemical methods. Chemical Society Reviews, 2012, 41, 3119.	38.1	60
74	Explicitly correlated benchmark calculations on C_8H_8 isomer energy separations: how accurate are DFT, double-hybrid, and composite <i>ab initio</i> procedures? Molecular Physics, 2012, 110, 2477-2491.	1.7	63
75	Spin-component-scaled electron correlation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 886-906.	14.6	197
76	Accurate and fast treatment of large molecular systems: Assessment of CEPA and pCCSD within the local pair natural orbital approximation. Journal of Computational Chemistry, 2012, 33, 2067-2072.	3.3	12
77	Accurate Computation of Structures and Strain Energies of Cyclophanes with Modern DFT Methods. Israel Journal of Chemistry, 2012, 52, 180-192.	2.3	38
78	Nanodiamonds in sugar rings: an experimental and theoretical investigation of cyclodextrin-nanodiamond inclusion complexes. Organic and Biomolecular Chemistry, 2012, 10, 4524.	2.8	50
80	Hydrogen Abstraction Reactivity Patterns from A...to...Y: The Valence Bond Way. Angewandte Chemie - International Edition, 2012, 51, 5556-5578.	13.8	233
81	Supramolecular Binding Thermodynamics by Dispersion-Corrected Density Functional Theory. Chemistry - A European Journal, 2012, 18, 9955-9964.	3.3	1,346
82	Gas-Phase Thermodynamics as a Validation of Computational Catalysis on Surfaces: A Case Study of Fischer-Tropsch Synthesis. ChemPhysChem, 2012, 13, 1486-1494.	2.1	23
83	Comment on: "On the Accuracy of DFT Methods in Reproducing Ligand Substitution Energies for Transition Metal Complexes in Solution: The Role of Dispersive Interactions" by H. Jacobsen and L. Cavallo. ChemPhysChem, 2012, 13, 1407-1409.	2.1	42
84	Accurate thermochemistry from a parameterized coupled-cluster singles and doubles model and a local pair natural orbital based implementation for applications to larger systems. Journal of Chemical Physics, 2012, 136, 064101.	3.0	68
85	Blind prediction of host-guest binding affinities: a new SAMPL3 challenge. Journal of Computer-Aided Molecular Design, 2012, 26, 475-487.	2.9	117

#	ARTICLE	IF	CITATIONS
86	Extending the applicability of the PBE0-DH double-hybrid model to weak interactions. <i>Chemical Physics Letters</i> , 2012, 535, 136-139.	2.6	10
87	Testing the broad applicability of the PBEint GGA functional and its one-parameter hybrid form. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 673-682.	2.0	33
88	Effects of London dispersion correction in density functional theory on the structures of organic molecules in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16031.	2.8	238
89	Mechanistic aspects of the reaction of dimerone derivatives with sulfenic acids and other sulfur compounds—a computational study. <i>Tetrahedron</i> , 2013, 69, 7243-7252.	1.9	7
90	Attenuated second-order Møller-Plesset perturbation theory: performance within the aug-cc-pVTZ basis. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15869.	2.8	44
91	Nonlocal van der Waals Approach Merged with Double-Hybrid Density Functionals: Toward the Accurate Treatment of Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3437-3443.	5.3	53
92	Accuracy of Quantum Chemical Methods for Large Noncovalent Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3364-3374.	5.3	275
93	Recent Progress in Density Functional Methodology for Biomolecular Modeling. <i>Structure and Bonding</i> , 2013, , 1-64.	1.0	9
94	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. , 2013, , 1-57.		1
95	Spin-component-scaled double hybrids: An extensive search for the best fifth-generation functionals blending DFT and perturbation theory. <i>Journal of Computational Chemistry</i> , 2013, 34, 2327-2344.	3.3	292
96	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 355-363.	5.3	68
97	Performance of Density Functionals for Activation Energies of Zr-Mediated Reactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4735-4743.	5.3	62
98	Estimating Chloride Polarizability in a Water Solution. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3221-3226.	2.5	8
99	Performance of M06, M06-2X, and M06-HF Density Functionals for Conformationally Flexible Anionic Clusters: M06 Functionals Perform Better than B3LYP for a Model System with Dispersion and Ionic Hydrogen-Bonding Interactions. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12590-12600.	2.5	549
101	Assessing the performances of some recently proposed density functionals for the description of organometallic structures. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	1.4	12
102	Coordination of CO to low-valent phosphorus centres and other related P=C bonding situations. A theoretical case study. <i>Chemical Science</i> , 2013, 4, 4309.	7.4	27
103	Quantum Chemical Challenges for the Binding of Simple Alkanes to Supramolecular Hosts. <i>Journal of Physical Chemistry B</i> , 2013, 117, 13409-13417.	2.6	24
104	Double-hybrid density functionals: merging wavefunction and density approaches to get the best of both worlds. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14581.	2.8	100

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105	Benchmark Study of the Performance of Density Functional Theory for Bond Activations with (Ni,Pd)-Based Transition-Metal Catalysts. <i>ChemistryOpen</i> , 2013, 2, 115-124.	1.9	146
106	A Systematic Approach to Identify Cooperatively Bound Homotrimers. <i>Journal of Physical Chemistry A</i> , 2013, 117, 174-182.	2.5	18
107	Parametrization and Benchmark of DFTB3 for Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 338-354.	5.3	743
108	Assessment of a Nonlocal Correction Scheme to Semilocal Density Functional Theory Methods. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 273-283.	5.3	27
109	The Lewis Acidity of the BO Triple Bond in Methyl(oxo)-borane. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2013, 639, 1199-1204.	1.2	2
110	New steroidal 7-azaindole platinum(II) antitumor complexes. <i>Journal of Inorganic Biochemistry</i> , 2013, 128, 48-56.	3.5	24
111	Torsional barriers of substituted biphenyls calculated using density functional theory: a benchmarking study. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 2859.	2.8	51
112	Are DFT Methods Accurate in Mononuclear Ruthenium-Catalyzed Water Oxidation? An ab Initio Assessment. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1872-1879.	5.3	43
113	Performance of Non-Local and Atom-Pairwise Dispersion Corrections to DFT for Structural Parameters of Molecules with Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 308-315.	5.3	91
114	A Benchmark Ab Initio and DFT Study of the Structure and Binding of Methane in the η^5 -Alkane Complex $\text{CpRe}(\text{CO})_2(\text{CH}_4)$. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2199-2208.	5.3	39
115	Accurate quantum chemical energies for tetrapeptide conformations: why MP2 data with an insufficient basis set should be handled with caution. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7028.	2.8	67
116	What Can We Learn about Dispersion from the Conformer Surface of <i>n</i> -Pentane?. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3118-3132.	2.5	60
117	Benchmark quantum-chemical calculations on a complete set of rotameric families of the DNA sugar-phosphate backbone and their comparison with modern density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7295.	2.8	33
118	Efficient Methods for the Quantum Chemical Treatment of Protein Structures: The Effects of London-Dispersion and Basis-Set Incompleteness on Peptide and Water-Cluster Geometries. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3240-3251.	5.3	75
119	Analytic Derivatives of Quartic-Scaling Doubly Hybrid XYGJ-OS Functional: Theory, Implementation, and Benchmark Comparison with M06-2X and MP2 Geometries for Nonbonded Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1971-1976.	5.3	15
120	Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. <i>Journal of Computational Chemistry</i> , 2013, 34, 1759-1774.	3.3	26
121	Water 16-mers and Hexamers: Assessment of the Three-Body and Electrostatically Embedded Many-Body Approximations of the Correlation Energy or the Nonlocal Energy As Ways to Include Cooperative Effects. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4486-4499.	2.5	30
122	Electron Correlation in the Condensed Phase from a Resolution of Identity Approach Based on the Gaussian and Plane Waves Scheme. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2654-2671.	5.3	113

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123	Intermolecular interactions of formic acid with benzene: Energy decomposition analyses with <i>ab initio</i> MP2 and double-hybrid density functional computations. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2355-2360.	2.0	12
124	Obtaining the lattice energy of the anthracene crystal by modern yet affordable first-principles methods. <i>Journal of Chemical Physics</i> , 2013, 138, 204304.	3.0	17
125	Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1669-1675.	4.6	63
126	The Performance of Density Functionals for Sulfate-Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1368-1380.	5.3	69
127	Extension of the B3LYP-dispersion-correcting potential approach to the accurate treatment of both inter- and intra-molecular interactions. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	1.4	45
128	Conformational Analysis of Furanoside-Containing Mono- and Oligosaccharides. <i>Chemical Reviews</i> , 2013, 113, 1851-1876.	47.7	117
129	A comparison of geometric parameters from PBE-based doubly hybrid density functionals PBE0-DH, PBE0-2, and xDH-PBE0. <i>Journal of Chemical Physics</i> , 2013, 139, 174106.	3.0	32
130	Thermal conductivity of argon at high pressure from first principles calculations. <i>Journal of Applied Physics</i> , 2013, 114, 064902.	2.5	14
131	Theoretical investigation on the 2e/12c bond and second hyperpolarizability of azaphenalenyl radical dimers: Strength and effect of dimerization. <i>Journal of Chemical Physics</i> , 2013, 139, 124314.	3.0	13
132	Efficient distance-including integral screening in linear-scaling Møller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , 2013, 138, 014101.	3.0	66
133	Orbital optimized double-hybrid density functionals. <i>Journal of Chemical Physics</i> , 2013, 139, 024110.	3.0	67
135	The nature of excess electrons in anatase and rutile from hybrid DFT and RPA. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26144-26152.	2.8	95
136	Assessment of theoretical procedures for a diverse set of isomerization reactions involving double-bond migration in conjugated dienes. <i>Chemical Physics</i> , 2014, 441, 166-177.	1.9	49
137	Temporary anion states of p-benzoquinone: shape and core-excited resonances. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26306-26313.	2.8	16
138	Assessment of density-functionals for describing the $X^{\bullet} + CH_3ONO_2$ gas-phase reactions with $X = F, OH, CH_2CN$. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26769-26778.	2.8	11
139	Multifunctional Benzothiadiazole-Based Small Molecules Displaying Solvatochromism and Sensing Properties toward Nitroarenes, Anions, and Cations. <i>ChemistryOpen</i> , 2014, 3, 242-249.	1.9	21
140	Pair-Potential Approach to Accurate Dispersion Energies between Group 12 (Zn, Cd, Hg) Clusters. <i>Journal of Physical Chemistry A</i> , 2014, 118, 12274-12279.	2.5	3
141	Origin of Inversion versus Retention in the Oxidative Addition of 3-Chloro-cyclopentene to $Pd(O)L_2$. <i>Journal of Organic Chemistry</i> , 2014, 79, 12136-12147.	3.2	17

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142	The 3-Acetyloxaphosphirane/1,3,2-Dioxaphosphol-4-ene Rearrangement. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 1727-1734.	2.0	11
143	How important is self-consistency for the dDsC density dependent dispersion correction?. <i>Journal of Chemical Physics</i> , 2014, 140, 18A516.	3.0	24
144	Unveiling the mechanism of selective gate-driven diffusion of CO ₂ over N ₂ in MFU-4 metal-organic framework. <i>Dalton Transactions</i> , 2014, 43, 9612-9619.	3.3	22
145	Dispersion-correcting potentials can significantly improve the bond dissociation enthalpies and noncovalent binding energies predicted by density-functional theory. <i>Journal of Chemical Physics</i> , 2014, 140, 18A542.	3.0	23
146	Intermolecular symmetry-adapted perturbation theory study of large organic complexes. <i>Journal of Chemical Physics</i> , 2014, 141, 094107.	3.0	77
147	Communication: Double-hybrid functionals from adiabatic-connection: The QIDH model. <i>Journal of Chemical Physics</i> , 2014, 141, 031101.	3.0	154
148	Large Nonlinear Optical Responses of Dimers Bearing a Donor and Acceptor: Long, Intradimer Multicenter Bonding. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28746-28756.	3.1	37
149	Density functional theory approach to gold-ligand interactions: Separating true effects from artifacts. <i>Journal of Chemical Physics</i> , 2014, 140, 244313.	3.0	14
150	Computational Approaches to Homogeneous Gold Catalysis. <i>Topics in Current Chemistry</i> , 2014, 357, 213-283.	4.0	28
151	Accurate Structure and Bonding Description of the Transition Metal Disulfur Monoxide Complexes [(PMe ₃) ₂ M(S ₂ O)] (M = Ni, Pd, Pt): Grimme Dispersion Corrected DFT Study. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2014, 640, 370-379.	1.2	2
152	The Ring and Exchange-Ring Approximations Based on Kohn-Sham Reference States. <i>Topics in Current Chemistry</i> , 2014, , 97-144.	4.0	3
153	The polymerisation of oligo(ethylene glycol methyl ether) methacrylate from a multifunctional poly(ethylene imine) derived amide: a stabiliser for the synthesis and dispersion of magnetite nanoparticles. <i>Polymer Chemistry</i> , 2014, 5, 524-534.	3.9	12
154	Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2014, 372, 20120476.	3.4	599
155	How Do DFT-DCP, DFT-NL, and DFT-D3 Compare for the Description of London-Dispersion Effects in Conformers and General Thermochemistry?. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 968-980.	5.3	81
156	Accurate quadruple- η basis-set approximation for double-hybrid density functional theory with an order of magnitude reduction in computational cost. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	18
158	Phenol-Quinone Tautomerism in (Arylazo)naphthols and the Analogous Schiff Bases: Benchmark Calculations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 778-789.	2.5	23
159	Developments in Theoretical Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 895-896.	5.3	0
160	Perspective: Fifty years of density-functional theory in chemical physics. <i>Journal of Chemical Physics</i> , 2014, 140, 18A301.	3.0	1,083

#	ARTICLE	IF	CITATIONS
161	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. Topics in Current Chemistry, 2014, , 1-23.	4.0	17
162	A DFT study on a mutipathways, one product reaction: Initially divergent radical reactions reconverge to form a single product. International Journal of Quantum Chemistry, 2014, 114, 769-781.	2.0	1
163	Double-Hybrid Density Functionals Free of Dispersion and Counterpoise Corrections for Non-Covalent Interactions. Journal of Physical Chemistry A, 2014, 118, 3175-3182.	2.5	23
164	Construction of a parameter-free doubly hybrid density functional from adiabatic connection. Journal of Chemical Physics, 2014, 140, 18A512.	3.0	57
165	What are the spectroscopic properties of HFC-32? Answers from DFT. International Journal of Quantum Chemistry, 2014, 114, 1472-1485.	2.0	16
166	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.	5.3	34
168	A New-Generation Density Functional. Springer Briefs in Molecular Science, 2014, , .	0.1	20
169	Searching for the thermodynamic limit â€“ a DFT study of the step-wise water oxidation of the bipyramidal Cu₇ cluster. Physical Chemistry Chemical Physics, 2014, 16, 2452-2464.	2.8	24
170	Computational Chemistry Meets Experiments for Explaining the Behavior of Bibenzyl: A Thermochemical and Spectroscopic (Infrared, Raman, and NMR) Investigation. Journal of Chemical Theory and Computation, 2014, 10, 5586-5592.	5.3	22
171	The MC-DFT approach including the SCS-MP2 energies to the new minnesota-type functionals. Journal of Computational Chemistry, 2014, 35, 1560-1567.	3.3	4
172	The Thermochemistry of London Dispersionâ€Driven Transition Metal Reactions: Getting the â€Right Answer for the Right Reasonâ€™. ChemistryOpen, 2014, 3, 177-189.	1.9	77
173	Quantum Chemical Investigations on Molecular Clusters. Chemical Reviews, 2014, 114, 12132-12173.	47.7	170
174	Benchmarking Calculated Lattice Parameters and Energies of Molecular Crystals Using van der Waals Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3423-3437.	5.3	56
175	Insights into the nature of Mâ€E bonds in [(PMe3)4Mâ€E(Mes)]+ (M = Mo, W) and [(PMe3)5Wâ€E(Mes)]+: a dispersion-corrected DFT study. RSC Advances, 2014, 4, 13034.	3.6	4
176	Dissociative electron attachment to the complexation ligands hexafluoroacetylacetone, trifluoroacetylacetone and acetylacetone; a comparative experimental and theoretical study. RSC Advances, 2014, 4, 33222-33235.	3.6	11
177	From Molecules to Materials: Computational Design of Nâ€Containing Porous Aromatic Frameworks for CO₂ Capture. ChemPhysChem, 2014, 15, 1772-1778.	2.1	11
178	Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 3669-3680.	5.3	334
179	Performance of Density Functionals for Activation Energies of Re-Catalyzed Organic Reactions. Journal of Chemical Theory and Computation, 2014, 10, 579-588.	5.3	47

#	ARTICLE	IF	CITATIONS
180	Developments in Theoretical Chemistry. Journal of Physical Chemistry A, 2014, 118, 1759-1760.	2.5	0
181	Some Observations on Counterpoise Corrections for Explicitly Correlated Calculations on Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 3791-3799.	5.3	109
182	Analysis of the structure and morphology of fenoxycarb crystals. Journal of Molecular Graphics and Modelling, 2014, 53, 92-99.	2.4	6
183	Energies and 2 π -Hydroxyl Group Orientations of RNA Backbone Conformations. Benchmark CCSD(T)/CBS Database, Electronic Analysis, and Assessment of DFT Methods and MD Simulations. Journal of Chemical Theory and Computation, 2014, 10, 463-480.	5.3	24
184	Benchmark Study on Methanol C-H and O-H Bond Activation by Bare [Fe ^{IV} O ₂] ²⁺ . Journal of Physical Chemistry A, 2014, 118, 7146-7158.	2.5	30
185	Double-hybrid density functionals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 576-600.	14.6	292
187	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.	5.3	44
188	Crystal Packing Induced Carbon-Carbon Double-Triple Bond Isomerization in a Zirconocene Complex. Organometallics, 2014, 33, 5358-5364.	2.3	12
189	Spin-Component-Scaled Double-Hybrid Density Functionals with Nonlocal van der Waals Correlations for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 4400-4407.	5.3	39
190	QM Computations on Complete Nucleic Acids Building Blocks: Analysis of the Sarcin-Ricin RNA Motif Using DFT-D3, HF-3c, PM6-D3H, and MM Approaches. Journal of Chemical Theory and Computation, 2014, 10, 2615-2629.	5.3	32
191	Novel Recipe for Double-Hybrid Density Functional Computations of Linear and Nonlinear Polarizabilities of Molecules and Nanoclusters. Journal of Physical Chemistry A, 2014, 118, 5333-5342.	2.5	20
192	Performance of recent density functionals to discriminate between olefin and nitrogen binding to palladium. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	7
193	Fractional Charge Behavior and Band Gap Predictions with the XYG3 Type of Doubly Hybrid Density Functionals. Journal of Physical Chemistry A, 2014, 118, 9201-9211.	2.5	45
194	At What Chain Length Do Unbranched Alkanes Prefer Folded Conformations?. Journal of Physical Chemistry A, 2014, 118, 1706-1712.	2.5	64
195	New Benchmark Set of Transition-Metal Coordination Reactions for the Assessment of Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3092-3103.	5.3	181
196	Wavefunction and reactivity study of benzo[a]pyrene diol epoxide and its enantiomeric forms. Structural Chemistry, 2014, 25, 1521-1533.	2.0	370
197	Inversion and rotation processes involving non-planar aromatic compounds catalyzed by extended polycyclic aromatic hydrocarbons. Chemical Physics Letters, 2014, 614, 156-161.	2.6	22
198	Correlated Ab Initio and Density Functional Studies on H ₂ Activation by FeO ⁺ . Journal of Chemical Theory and Computation, 2014, 10, 3807-3820.	5.3	95

#	ARTICLE	IF	CITATIONS
217	Stimuli-Responsive Frustrated Lewis Pair-Type Reactivity of a Tungsten Iminoazaphosphiridine Complex. Chemistry - A European Journal, 2015, 21, 9650-9655.	3.3	20
218	Benchmarking DFT and semiempirical methods on structures and lattice energies for ten ice polymorphs. Journal of Chemical Physics, 2015, 142, 124104.	3.0	84
219	A Preorganized Ditopic Borane as Highly Efficient One- or Two-Electron Trap. Journal of the American Chemical Society, 2015, 137, 3705-3714.	13.7	90
220	Theoretical insights into structure, bonding, reactivity and importance of ion-pair interactions in Kirby's tetrafluoroboric acid salts of twisted amides. RSC Advances, 2015, 5, 105668-105677.	3.6	2
221	CYANOMETHANIMINE ISOMERS IN COLD INTERSTELLAR CLOUDS: INSIGHTS FROM ELECTRONIC STRUCTURE AND KINETIC CALCULATIONS. Astrophysical Journal, 2015, 810, 111.	4.5	53
222	Relative energies of water nanoclusters (H ₂ O) ₂₀ : comparison of empirical and nonempirical double-hybrids with generalized energy-based fragmentation approach. New Journal of Chemistry, 2015, 39, 5534-5539.	2.8	13
223	Benchmarking Ground-State Geometries and Vertical Excitation Energies of a Selection of P-Type Semiconducting Molecules with Different Polarity. Journal of Physical Chemistry A, 2015, 119, 12876-12891.	2.5	25
224	The Nonlocal Correlation Density Functional VV10. Annual Reports in Computational Chemistry, 2015, 11, 37-102.	1.7	17
225	Negative hyperconjugation and red-, blue- or zero-shift in X ⁺ ⋯Z ⁻ Y complexes. Faraday Discussions, 2015, 177, 33-50.	3.2	20
226	Further evidences on the quality of meta-GGA linearly scaled one-parameter double-hybrids for frontier orbital energies. Chemical Physics Letters, 2015, 623, 14-16.	2.6	9
227	Stacking of Metal Chelates with Benzene: Can Dispersion-Corrected DFT Be Used to Calculate Organic-Inorganic Stacking?. ChemPhysChem, 2015, 16, 761-768.	2.1	14
228	Reassessment of the Thermodynamic, Kinetic, and Spectroscopic Features of Cyanomethanimine Derivatives: A Full Anharmonic Perturbative Treatment. Journal of Chemical Theory and Computation, 2015, 11, 1165-1171.	5.3	19
229	Accurate reaction barrier heights of pericyclic reactions: Surprisingly large deviations for the CBS-QB3 composite method and their consequences in DFT benchmark studies. Journal of Computational Chemistry, 2015, 36, 622-632.	3.3	124
230	Activation of C-H and B-H bonds through agostic bonding: an ELF/QTAIM insight. Physical Chemistry Chemical Physics, 2015, 17, 9258-9281.	2.8	36
231	Basis set limit coupled-cluster studies of hydrogen-bonded systems. Molecular Physics, 2015, 113, 1618-1629.	1.7	24
232	Comparative Assessment of DFT Performances in Ru- and Rh-Promoted Ĩf-Bond Activations. Journal of Chemical Theory and Computation, 2015, 11, 1428-1438.	5.3	45
233	Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. Journal of Chemical Theory and Computation, 2015, 11, 1525-1539.	5.3	544
234	Reaction barrier heights for cycloreversion of heterocyclic rings: An Achilles' heel for DFT and standard ab initio procedures. Chemical Physics, 2015, 458, 1-8.	1.9	68

#	ARTICLE	IF	CITATIONS
235	Dissociative electron attachment to bromotrifluoromethane. International Journal of Mass Spectrometry, 2015, 387, 78-82.	1.5	1
236	Reformulation of the D3(Beckeâ€Johnson) Dispersion Correction without Resorting to Higher than C_{6D} Dispersion Coefficients. Journal of Chemical Theory and Computation, 2015, 11, 3163-3170.	5.3	83
237	Accurate Dielsâ€Alder Reaction Energies from Efficient Density Functional Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2879-2888.	5.3	19
238	Influence of solvent on crystal nucleation of risperidone. Faraday Discussions, 2015, 179, 309-328.	3.2	62
239	Designing a paradigm for parameter-free double-hybrid density functionals through the adiabatic connection path. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	26
240	Is It Possible To Obtain Coupled Cluster Quality Energies at near Density Functional Theory Cost? Domain-Based Local Pair Natural Orbital Coupled Cluster vs Modern Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 4054-4063.	5.3	248
241	Mechanism and Selectivity in Rhodium-Catalyzed [7 + 2] Cycloaddition and Cyclopropanation/Cyclization of Allenylcyclopentane-alkynes: Metallacycle-Directed $C(sp^3)-C(sp^3)$ vs $C(sp^3)-H$ Activation. Journal of Organic Chemistry, 2015, 80, 7564-7571.	3.2	29
242	Dispersion Corrections Improve the Accuracy of Both Noncovalent and Covalent Interactions Energies Predicted by a Density-Functional Theory Approximation. Journal of Physical Chemistry A, 2015, 119, 6703-6713.	2.5	27
243	Photoisomerization action spectroscopy: flicking the protonated merocyanineâ€spiropyran switch in the gas phase. Physical Chemistry Chemical Physics, 2015, 17, 25676-25688.	2.8	46
244	Hydration Enthalpies of $Ba^{2+}(H_2O)_2$, $x = 1-8$: A Threshold Collision-Induced Dissociation and Computational Investigation. Journal of Physical Chemistry A, 2015, 119, 3800-3815.	2.5	21
245	Quantum-Chemical Characterization of the Properties and Reactivities of Metalâ€Organic Frameworks. Chemical Reviews, 2015, 115, 6051-6111.	47.7	241
246	Homogeneous Catalysis with Au^{III} : Insights into the Mechanism of the Alkoxylation of Alkynes. European Journal of Inorganic Chemistry, 2015, 2015, 2381-2386.	2.0	2
247	A quest for stable 2,5-bis(halobora)cyclopentenylidene and its Si, Ge, Sn and Pb analogs at theoretical levels. RSC Advances, 2015, 5, 43319-43327.	3.6	18
248	Mapping the genome of meta-generalized gradient approximation density functionals: The search for B97M-V. Journal of Chemical Physics, 2015, 142, 074111.	3.0	305
249	Synthesis, crystal structure, theoretical calculations, and electrochemical and biological studies of polymeric $(N,N,N',N''\text{-tetramethylethylenediamine})\text{bis}(\text{thiocyanato-}\lambda^1\text{N})\text{copper(II)}$, $[Cu(\text{tmeda})(\text{NCS})_2]_n$. Polyhedron, 2015, 90, 252-257.	2.2	16
250	Communication: A new class of non-empirical explicit density functionals on the third rung of Jacobâ€™s ladder. Journal of Chemical Physics, 2015, 143, 111105.	3.0	13
251	Gas-phase formation of the prebiotic molecule formamide: insights from new quantum computations. Monthly Notices of the Royal Astronomical Society: Letters, 2015, 453, L31-L35.	3.3	131
252	Physicochemical mechanisms of plasma-liquid interactions within plasma channels in liquid. Journal Physics D: Applied Physics, 2015, 48, 424004.	2.8	19

#	ARTICLE	IF	CITATIONS
253	Three-Coordinate Iron(IV) Bisimido Complexes with Aminocarbene Ligation: Synthesis, Structure, and Reactivity. <i>Journal of the American Chemical Society</i> , 2015, 137, 14196-14207.	13.7	88
254	A multi-scale approach to characterize pure CH ₄ , CF ₄ , and CH ₄ /CF ₄ mixtures. <i>Journal of Chemical Physics</i> , 2015, 142, 164508.	3.0	8
255	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. <i>Journal of Chemical Physics</i> , 2015, 143, 054107.	3.0	605
256	The propargylbenzene dimer: C π -H π assisted π - π stacking. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9090-9097.	2.8	15
257	Assessment of DFT Methods for Computing Activation Energies of Mo/W-Mediated Reactions. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4601-4614.	5.3	52
258	Construction and Application of a New Dual-Hybrid Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4615-4626.	5.3	54
259	Quantum Chemical Benchmark Study on 46 RNA Backbone Families Using a Dinucleotide Unit. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4972-4991.	5.3	90
260	Theoretical insights into M-SO bonds in transition metal-sulfur monoxide complexes [{N(SPM ₂) ₂ } ₂ M(SO)] (M = Fe, Ru, Os): Assessment of density functionals and dispersion interactions. <i>Polyhedron</i> , 2015, 101, 230-238.	2.2	8
261	Importance of the Electron Correlation and Dispersion Corrections in Calculations Involving Enamines, Hemiaminals, and Amins. Comparison of B3LYP, M06-2X, MP2, and CCSD Results with Experimental Data. <i>Journal of Organic Chemistry</i> , 2015, 80, 11977-11985.	3.2	27
262	Toward the construction of parameter-free doubly hybrid density functionals. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 589-595.	2.0	22
263	Validation of the Direct-COSMO-RS Solvent Model for Diels-Alder Reactions in Aqueous Solution. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 111-121.	5.3	13
264	Towards biochemically relevant QM computations on nucleic acids: controlled electronic structure geometry optimization of nucleic acid structural motifs using penalty restraint functions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 1399-1410.	2.8	25
265	An assessment of theoretical procedures for π -conjugation stabilisation energies in enones. <i>Molecular Physics</i> , 2015, 113, 1284-1296.	1.7	19
266	Local response dispersion method: A density-dependent dispersion correction for density functional theory. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 309-324.	2.0	12
267	Non-parametrized functionals with empirical dispersion corrections: A happy match?. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	16
268	Local response dispersion method in periodic systems: Implementation and assessment. <i>Journal of Computational Chemistry</i> , 2015, 36, 303-311.	3.3	4
269	Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution. <i>Computer Physics Communications</i> , 2015, 187, 120-129.	7.5	42
270	Accurate, Precise, and Efficient Theoretical Methods To Calculate Anion- π Interaction Energies in Model Structures. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 360-371.	5.3	26

#	ARTICLE	IF	CITATIONS
271	Analytical Double-Hybrid Density Functional Based on the Polynomial Series Expansion of Adiabatic Connection: A Quadratic Approximation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 45-54.	5.3	22
272	Spectroscopic and ab initio investigation of 2,6-difluorophenylacetylene-amine complexes: coexistence of C-H...N and lone-pair...F complexes and intermolecular coulombic decay. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 434-443.	2.8	14
273	On the Use of Benchmarks for Multiple Properties. <i>Computation</i> , 2016, 4, 20.	2.0	7
274	Towards a barrier height benchmark set for biologically relevant systems. <i>PeerJ</i> , 2016, 4, e1994.	2.0	22
276	Comparison of one-parameter and linearly scaled one-parameter double-hybrid density functionals for noncovalent interactions. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1166-1172.	2.0	5
277	Order of stabilities in water nanoclusters: Insight from some recent double-hybrid functionals. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1173-1178.	2.0	0
278	Predictive coupled-cluster isomer orderings for some Si_nC_m (_n, _m ≤ 12) clusters: A pragmatic comparison between DFT and complete basis limit coupled-cluster benchmarks. <i>Journal of Chemical Physics</i> , 2016, 145, 024312.	3.0	14
279	Self-consistent implementation of meta-GGA functionals for the ONETEP linear-scaling electronic structure package. <i>Journal of Chemical Physics</i> , 2016, 145, 204114.	3.0	18
280	Ionization potential optimized double-hybrid density functional approximations. <i>Journal of Chemical Physics</i> , 2016, 145, 104106.	3.0	17
281	Perspective: Kohn-Sham density functional theory descending a staircase. <i>Journal of Chemical Physics</i> , 2016, 145, 130901.	3.0	243
282	Spin polarization in SCC-DFTB. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	9
283	Molecular energies from an incremental fragmentation method. <i>Journal of Chemical Physics</i> , 2016, 144, 084109.	3.0	21
284	B97M-V: A combinatorially optimized, range-separated hybrid, meta-GGA density functional with VV10 nonlocal correlation. <i>Journal of Chemical Physics</i> , 2016, 144, 214110.	3.0	595
285	Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept, and a pilot implementation. <i>Journal of Chemical Physics</i> , 2016, 145, 044109.	3.0	16
286	Ability of density functional theory methods to accurately model the reaction energy pathways of the oxidation of CO on gold cluster: A benchmark study. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	11
287	A dataset of highly accurate homolytic Ni-Br bond dissociation energies obtained by Means of W2 theory. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 52-60.	2.0	28
288	New approaches for the calibration of exchange-energy densities in local hybrid functionals. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21133-21144.	2.8	43
289	Comparison of Three Efficient Approximate Exact-Exchange Algorithms: The Chain-of-Spheres Algorithm, Pair-Atomic Resolution-of-the-Identity Method, and Auxiliary Density Matrix Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3514-3522.	5.3	29

#	ARTICLE	IF	CITATIONS
290	Structural and relative energy assessments of DFT functionals and the MP2 method to describe the gas phase methylation of nitronates: $[R^{1+}R^{2+}CNO^{2-}]^{+} + CH_3I$. Physical Chemistry Chemical Physics, 2016, 18, 17062-17070.	2.8	11
291	Structure of isothiocyanic acid dimers. Theoretical and FTIR matrix isolation studies. Chemical Physics Letters, 2016, 652, 46-49.	2.6	6
292	Exchange-Correlation Functionals via Local Interpolation along the Adiabatic Connection. Journal of Chemical Theory and Computation, 2016, 12, 2598-2610.	5.3	40
293	Systematic Error Estimation for Chemical Reaction Energies. Journal of Chemical Theory and Computation, 2016, 12, 2762-2773.	5.3	71
294	Screened exchange hybrid density functional for accurate and efficient structures and interaction energies. Physical Chemistry Chemical Physics, 2016, 18, 15519-15523.	2.8	49
295	DFT Methods to Study the Reaction Mechanism of Iridium-Catalyzed Hydrogenation of Olefins: Which Functional Should be Chosen?. ChemPhysChem, 2016, 17, 119-127.	2.1	14
296	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. Chemical Reviews, 2016, 116, 5301-5337.	47.7	312
297	Dispersion-Corrected Mean-Field Electronic Structure Methods. Chemical Reviews, 2016, 116, 5105-5154.	47.7	1,032
298	The nature of M-PNR ₂ bonds in the electrophilic phosphinidene complexes $[(L)(CO)_3M\{PNR_2\}]^+$ (L = Tj ETQqO O O rgBT /Overlock 10 Tj). Organometallic Chemistry, 2016, 813, 84-94.	1.8	3
299	Seeking for Spin-Opposite-Scaled Double-Hybrid Models Free of Fitted Parameters. Journal of Physical Chemistry A, 2016, 120, 3726-3730.	2.5	28
300	Implementation of Molecular Gradients for Local Hybrid Density Functionals Using Seminumerical Integration Techniques. Journal of Chemical Theory and Computation, 2016, 12, 4254-4262.	5.3	33
301	Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. Chemical Communications, 2016, 52, 13840-13860.	4.1	18
302	State-of-the-Art Thermochemical and Kinetic Computations for Astrochemical Complex Organic Molecules: Formamide Formation in Cold Interstellar Clouds as a Case Study. Journal of Chemical Theory and Computation, 2016, 12, 5385-5397.	5.3	56
303	Comparative Assessment of Different RNA Tetranucleotides from the DFT-D3 and Force Field Perspective. Journal of Physical Chemistry B, 2016, 120, 10635-10648.	2.6	16
304	Frequency Scale Factors for Some Double-Hybrid Density Functional Theory Procedures: Accurate Thermochemical Components for High-Level Composite Protocols. Journal of Chemical Theory and Computation, 2016, 12, 3774-3780.	5.3	50
305	New aspects of UV photolysis of hydrogen peroxide. Nitrogen matrix isolation FTIR and theoretical studies. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 330, 134-139.	3.9	6
306	The INV24 test set: how well do quantum-chemical methods describe inversion and racemization barriers?. Canadian Journal of Chemistry, 2016, 94, 1133-1143.	1.1	45
307	Theoretical predication for transition energies of thermally activated delayed fluorescence molecules. Chinese Chemical Letters, 2016, 27, 1445-1452.	9.0	37

#	ARTICLE	IF	CITATIONS
308	How Accurate Are the Minnesota Density Functionals for Noncovalent Interactions, Isomerization Energies, Thermochemistry, and Barrier Heights Involving Molecules Composed of Main-Group Elements?. Journal of Chemical Theory and Computation, 2016, 12, 4303-4325.	5.3	355
309	Deprotonated guanine-cytosine and 9-methylguanine-cytosine base pairs and their non-statistical kinetics: a combined guided-ion beam and computational study. Physical Chemistry Chemical Physics, 2016, 18, 32222-32237.	2.8	17
310	Highly conductive and flexible fiber for textile electronics obtained by extremely low-temperature atomic layer deposition of Pt. NPG Asia Materials, 2016, 8, e331-e331.	7.9	51
311	Subtle solvation behaviour of a biofuel additive: the methanol complex with 2,5-dimethylfuran. Physical Chemistry Chemical Physics, 2016, 18, 27265-27271.	2.8	20
312	Structure and internal rotation dynamics of the acetone-neon complex studied by microwave spectroscopy. Journal of Molecular Spectroscopy, 2016, 330, 228-235.	1.2	3
313	Thiaphosphiranes and Their Complexes: Systematic Study on Ring Strain and Ring Cleavage Reactions. Inorganic Chemistry, 2016, 55, 9611-9619.	4.0	19
314	Activation of C-H Bonds in Pt+ + x CH4 Reactions, where x = 1-4: Identification of the Platinum Dimethyl Cation. Journal of Physical Chemistry A, 2016, 120, 6216-6227.	2.5	41
315	Does hydrohalic acid HX (X = F, Cl) form true N-protonated twisted amide salts? Effects of anions on the ion-pair interactions and on the amide moiety in N-protonated tricyclic twisted amide salts. New Journal of Chemistry, 2016, 40, 7831-7839.	2.8	1
316	Spherical conformational landscape shed new lights on fluxional nature of cyclopentane and its derivatives, confirmed by their Raman spectra. Computational and Theoretical Chemistry, 2016, 1090, 193-202.	2.5	8
317	The <sc>XYG3</sc> type of doubly hybrid density functionals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 721-747.	14.6	52
318	Regioselective Transition-Metal-Free Allyl-Allyl Cross-Couplings. Angewandte Chemie - International Edition, 2016, 55, 10502-10506.	13.8	19
319	A homoleptic, all-alkynyl-stabilized highly luminescent Au ₈ Ag ₈ cluster with a single crystal X-ray structure. Dalton Transactions, 2016, 45, 12772-12778.	3.3	18
320	Calculation of Electrochemical Energy Levels in Water Using the Random Phase Approximation and a Double Hybrid Functional. Physical Review Letters, 2016, 116, 086402.	7.8	38
321	Reparameterization of PM6 Applied to Organic Diradical Molecules. Journal of Physical Chemistry A, 2016, 120, 8750-8760.	2.5	16
322	Reactions of 2-Propanol Radical with Halogenated Organics in Aqueous Solution: Theoretical Evidence for Proton-Coupled Electron Transfer and Competing Mechanisms. Journal of Physical Chemistry B, 2016, 120, 11810-11820.	2.6	9
323	Benchmark tests of a strongly constrained semilocal functional with a long-range dispersion correction. Physical Review B, 2016, 94, .	3.2	152
324	Evaluation of the performance of MP4-based procedures for a wide range of thermochemical and kinetic properties. Chemical Physics, 2016, 480, 23-35.	1.9	8
325	Regioselective Allyl-Allyl Kreuzkupplungen ohne Übergangsmetallkatalysator. Angewandte Chemie, 2016, 128, 10658-10662.	2.0	8

#	ARTICLE	IF	CITATIONS
326	Quadratic integrand double-hybrid made spin-component-scaled. <i>Journal of Chemical Physics</i> , 2016, 144, 124104.	3.0	31
327	CuHâ€Catalysed Hydroamination of Styrene with Hydroxylamine Esters: A Coupled Cluster Scrutiny of Mechanistic Pathways. <i>Chemistry - A European Journal</i> , 2016, 22, 8290-8300.	3.3	44
328	Exchangeâ€Correlation Effects for Noncovalent Interactions in Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3160-3175.	5.3	24
329	Reactions of Li/Cl Phosphinidenoid Complexes with 1,3,4,5-Tetramethylimidazol-2-ylidene: A New Route to N-Heterocyclic Carbene Adducts of Terminal Phosphinidene Complexes and an Unprecedented Transformation of an Oxaphosphirane Complex. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 685-690.	2.0	21
330	On the inclusion of postâ€MP</sc>2 contributions to doubleâ€Hybrid density functionals. <i>Journal of Computational Chemistry</i> , 2016, 37, 183-193.	3.3	30
331	Noncatalytic bromination of benzene: A combined computational and experimental study. <i>Journal of Computational Chemistry</i> , 2016, 37, 210-225.	3.3	16
332	How Many Water Molecules Does it Take to Dissociate HCl?. <i>Chemistry - A European Journal</i> , 2016, 22, 2812-2818.	3.3	42
333	Gas phase enthalpies of formation, isomerization, and disproportionation of mono- through tetra-substituted tetrahydrides: A G4(MP2)/G4 theoretical study. <i>Computational and Theoretical Chemistry</i> , 2016, 1075, 30-37.	2.5	5
334	Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks for Ground-State Properties. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1097-1120.	5.3	74
335	The stacking interactions of bipyridine complexes: the influence of the metal ion type on the strength of interactions. <i>Journal of Molecular Modeling</i> , 2016, 22, 30.	1.8	7
336	From C₆₀ to Infinity: Large-Scale Quantum Chemistry Calculations of the Heats of Formation of Higher Fullerenes. <i>Journal of the American Chemical Society</i> , 2016, 138, 1420-1429.	13.7	32
337	Preferred Geometries and Energies of Sulfurâ€Sulfur Interactions in Crystal Structures. <i>Crystal Growth and Design</i> , 2016, 16, 632-639.	3.0	54
338	Theoretical study of the reactions of transition-metal monoxides (Scâ€V) with monochloromethane: Structures, energies and reaction mechanisms. <i>Computational and Theoretical Chemistry</i> , 2016, 1075, 1-8.	2.5	1
339	A computationally efficient double hybrid density functional based on the random phase approximation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20926-20937.	2.8	55
340	DFT/PCM theoretical study of the conversion of methyl 4-O-methyl-Î±-d-galactopyranoside 6-sulfate and its 2-sulfated derivative into their 3,6-anhydro counterparts. <i>Carbohydrate Research</i> , 2016, 426, 15-25.	2.3	3
341	Electron Detachment and Subsequent Structural Changes of Water Clusters. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1065-1073.	2.5	5
342	Importance of Orbital Optimization for Double-Hybrid Density Functionals: Application of the OO-PBE-QIDH Model for Closed- and Open-Shell Systems. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1756-1762.	2.5	31
343	Evaluation of Range-Corrected Density Functionals for the Simulation of Pyridinium-Containing Molecular Crystals. <i>Journal of Physical Chemistry A</i> , 2016, 120, 939-947.	2.5	23

#	ARTICLE	IF	CITATIONS
344	Gauge effects in local hybrid functionals evaluated for weak interactions and the GMTKN30 test set. <i>Molecular Physics</i> , 2016, 114, 1118-1127.	1.7	26
345	Development and Pharmacological Characterization of Selective Blockers of 2-Arachidonoyl Glycerol Degradation with Efficacy in Rodent Models of Multiple Sclerosis and Pain. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 2612-2632.	6.4	70
346	Rearrangement and deoxygenation of 3,3-bis(2-pyridyl)oxaphosphirane complexes. <i>Dalton Transactions</i> , 2016, 45, 2085-2094.	3.3	18
347	Derivation of Reliable Geometries in QM Calculations of DNA Structures: Explicit Solvent QM/MM and Restrained Implicit Solvent QM Optimizations of G-Quadruplexes. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2000-2016.	5.3	22
348	On the performance of time-dependent double-hybrid density functionals for description of absorption and emission spectra of heteroaromatic compounds. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	14
349	Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. <i>Chemical Reviews</i> , 2016, 116, 5038-5071.	47.7	346
350	Mechanistic Study of the Direct Intramolecular Allylic Amination Reaction Catalyzed by Palladium(II). <i>ACS Catalysis</i> , 2016, 6, 1772-1784.	11.2	21
351	CPh ₃ as a functional group in P-heterocyclic chemistry: elimination of HCPh ₃ in the reaction of P-CPh ₃ substituted Li/Cl phosphinidenoid complexes with Ph ₂ C=O. <i>Dalton Transactions</i> , 2016, 45, 2378-2385.	3.3	16
352	Î±-Hydrogen Abstraction by •COH and •CSH Radicals from Amino Acids and Their Peptide Derivatives. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1606-1613.	5.3	16
353	Redox potential tuning by redox-inactive cations in nature's water oxidizing catalyst and synthetic analogues. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10739-10750.	2.8	38
354	Benchmarking Density Functionals on Structural Parameters of Small-/Medium-Sized Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 459-465.	5.3	165
355	Buckminster fullerene adhesion on graphene flakes: Numerical accuracy of dispersion corrected DFT. <i>Polyhedron</i> , 2016, 114, 110-117.	2.2	8
356	Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. <i>Molecular Physics</i> , 2016, 114, 21-33.	1.7	21
357	Modelling of graphene functionalization. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6351-6372.	2.8	190
358	Long-range interactions from the many-pair expansion: A different avenue to dispersion in DFT. <i>Journal of Chemical Physics</i> , 2017, 146, 024111.	3.0	6
359	Formation Mechanisms of Naphthalene and Indene: From the Interstellar Medium to Combustion Flames. <i>Journal of Physical Chemistry A</i> , 2017, 121, 901-926.	2.5	130
360	DFT study of water adsorption on lignite molecule surface. <i>Journal of Molecular Modeling</i> , 2017, 23, 27.	1.8	30
361	The role of London dispersion interactions in strong and moderate intermolecular hydrogen bonds in the crystal and in the gas phase. <i>Chemical Physics Letters</i> , 2017, 672, 124-127.	2.6	11

#	ARTICLE	IF	CITATIONS
362	Computational study on vapor phase coupling reaction between diiso(thio)cyanates with diamines, diols, and dithiols. International Journal of Quantum Chemistry, 2017, 117, e25341.	2.0	2
363	Development of New Density Functional Approximations. Annual Review of Physical Chemistry, 2017, 68, 155-182.	10.8	51
364	Quantifying the efficiency of CO ₂ capture by Lewis pairs. Chemical Science, 2017, 8, 3270-3275.	7.4	36
365	Cu ^{II} TM: Promising catalysts for preferential oxidation of CO in H ₂ -rich gas. Computational and Theoretical Chemistry, 2017, 1105, 1-13.	2.5	2
366	The Borderline between Reactivity and Pre-reactivity of Binary Mixtures of Gaseous Carboxylic Acids and Alcohols. Angewandte Chemie - International Edition, 2017, 56, 3872-3875.	13.8	14
367	Competition of van der Waals and chemical forces on gold-sulfur surfaces and nanoparticles. Nature Reviews Chemistry, 2017, 1, .	30.2	95
368	Radical-polar crossover reactions of vinylboron ate complexes. Science, 2017, 355, 936-938.	12.6	227
369	Partnering dispersion corrections with modern parameter-free double-hybrid density functionals. Physical Chemistry Chemical Physics, 2017, 19, 13481-13487.	2.8	31
370	Benchmarking density functionals in conjunction with Grimme's dispersion correction for noble gas dimers (Ne ₂ , Ar ₂ , Kr ₂ , Xe ₂ ,) Tj ETQq0 0 0 rgBT / Overlock 102f 50 417		
371	Adsorption of carbon monoxide on the Si(111)-7 × 7 surface. Applied Surface Science, 2017, 405, 209-214.	6.1	4
372	Determining the role of the underlying orbital-dependence of PBE0-DH and PBE-QIDH double-hybrid density functionals. Journal of Computational Chemistry, 2017, 38, 1509-1514.	3.3	2
373	Assessing DFT-D3 Damping Functions Across Widely Used Density Functionals: Can We Do Better?. Journal of Chemical Theory and Computation, 2017, 13, 2043-2052.	5.3	71
374	Does the ionization potential condition employed in QTP functionals mitigate the self-interaction error?. Journal of Chemical Physics, 2017, 146, 034102.	3.0	22
375	Impact of Conjugation and Hyperconjugation on the Radical Stability of Allylic and Benzylic Systems: A Theoretical Study. Journal of Organic Chemistry, 2017, 82, 5731-5742.	3.2	9
376	Low scaling random-phase approximation electron correlation method including exchange interactions using localised orbitals. Journal of Chemical Physics, 2017, 146, 174110.	3.0	10
377	π-Stacked Dimers of Fluorophenylacetylenes: Role of Dipole Moment. Journal of Physical Chemistry A, 2017, 121, 3383-3391.	2.5	17
378	Benchmarking Quantum Chemical Methods: Are We Heading in the Right Direction?. Angewandte Chemie - International Edition, 2017, 56, 11011-11018.	13.8	119
379	A new near-linear scaling, efficient and accurate, open-shell domain-based local pair natural orbital coupled cluster singles and doubles theory. Journal of Chemical Physics, 2017, 146, 164105.	3.0	285

#	ARTICLE	IF	CITATIONS
380	Effect of dispersion corrections on covalent and non-covalent interactions in DFTB calculations. <i>Structural Chemistry</i> , 2017, 28, 1399-1407.	2.0	4
381	Revisiting the thermochemistry of chlorine fluorides. <i>Journal of Computational Chemistry</i> , 2017, 38, 1930-1940.	3.3	1
382	Gauging the performance of some density functionals including dispersion and nonlocal corrections for relative energies of water 20-mers. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 132-136.	2.4	3
383	Dissecting the accountability of parameterized and parameter-free single-hybrid and double-hybrid functionals for photophysical properties of TADF-based OLEDs. <i>Journal of Chemical Physics</i> , 2017, 146, 234304.	3.0	17
384	Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. <i>Molecular Physics</i> , 2017, 115, 2315-2372.	1.7	1,401
385	Atomic Layer Deposition of an Indium Gallium Oxide Thin Film for Thin-Film Transistor Applications. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 23934-23940.	8.0	97
386	Reaction mechanism, rate constants, and product yields for unimolecular and H-assisted decomposition of 2,4-cyclopentadienone and oxidation of cyclopentadienyl with atomic oxygen. <i>Combustion and Flame</i> , 2017, 183, 181-193.	5.2	32
387	Conventional and Explicitly Correlated ab Initio Benchmark Study on Water Clusters: Revision of the BEGDB and WATER27 Data Sets. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3136-3152.	5.3	81
388	Theoretical analysis of the binding of iron(III) protoporphyrin IX to 4-methoxyacetophenone thiosemicarbazone via DFT-D3, MEP, QTAIM, NCI, ELF, and LOL studies. <i>Journal of Molecular Modeling</i> , 2017, 23, 200.	1.8	81
389	Can DFT and ab initio methods adequately describe binding energies in strongly interacting C ₆ H ₆ ⋯C ₂ X ₂ complexes?. <i>Chemical Physics</i> , 2017, 493, 12-19.	1.9	7
390	The Borderline between Reactivity and Pre-reactivity of Binary Mixtures of Gaseous Carboxylic Acids and Alcohols. <i>Angewandte Chemie</i> , 2017, 129, 3930-3933.	2.0	6
391	Dimeric nature of N-coordinated Mg and Ca ions in metalloorganic compounds. The topological analysis of ELF functions for Mg⋯Mg and Ca⋯Ca bonds. <i>Polyhedron</i> , 2017, 129, 22-29.	2.2	6
392	What Can We Learn from a Biomimetic Model of Nature's Oxygen-Evolving Complex?. <i>Inorganic Chemistry</i> , 2017, 56, 3875-3888.	4.0	40
393	Automatic generation of reaction energy databases from highly accurate atomization energy benchmark sets. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 9798-9805.	2.8	30
394	Semilocal exchange hole with an application to range-separated density functionals. <i>Physical Review B</i> , 2017, 95, .	3.2	19
395	A Concise Synthesis of Presilphiperfolane Core through a Tandem TMTU⋯Co⋯Catalyzed Pauson⋯Khand Reaction and a 6π Electrocyclization Reaction (TMTU=Tetramethyl Thiourea). <i>Chemistry - A European Journal</i> , 2017, 23, 1258-1262.	3.3	23
396	Construction of a Spin-Component Scaled Dual-Hybrid Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 796-803.	5.3	25
397	A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32184-32215.	2.8	1,230

#	ARTICLE	IF	CITATIONS
398	Evaluation of the Factors Impacting the Accuracy of ^{13}C NMR Chemical Shift Predictions using Density Functional Theory—The Advantage of Long-Range Corrected Functionals. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5798-5819.	5.3	77
399	Theoretical investigation on the interaction of hypergolic monomethylhydrazine with 1-chloro-1,1-dinitro-2-(N-chloroamidino)ethane using DFT methods. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	0
400	Ethylene-Bridged Oligo-BODIPYs: Access to Intramolecular J-Aggregates and Superfluorophores. <i>Journal of the American Chemical Society</i> , 2017, 139, 15104-15113.	13.7	84
401	The short device lifetimes of blue PhOLEDs: insights into the photostability of blue Ir(III) complexes. <i>Chemical Science</i> , 2017, 8, 7844-7850.	7.4	76
402	The aug-cc-pVnZ-F12 basis set family: Correlation consistent basis sets for explicitly correlated benchmark calculations on anions and noncovalent complexes. <i>Journal of Chemical Physics</i> , 2017, 147, 134106.	3.0	50
403	Toward the Accurate Prediction of Liquid Phase Oxidation of Aromatics: A Detailed Kinetic Mechanism for Toluene Autoxidation. <i>Energy & Fuels</i> , 2017, 31, 12893-12913.	5.1	15
404	Benchmark Databases of Intermolecular Interaction Energies: Design, Construction, and Significance. <i>Annual Reports in Computational Chemistry</i> , 2017, 13, 3-91.	1.7	8
405	The BioFragment Database (BFDdb): An open-data platform for computational chemistry analysis of noncovalent interactions. <i>Journal of Chemical Physics</i> , 2017, 147, 161727.	3.0	82
406	General optimization procedure towards the design of a new family of minimal parameter spin-component-scaled double-hybrid density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26191-26200.	2.8	20
407	Rate constants for H abstraction from benzo(a)pyrene and chrysene: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25401-25413.	2.8	37
408	Role of dispersion corrected hybrid GGA class in accurately calculating the bond dissociation energy of carbon halogen bond: A benchmark study. <i>Journal of Molecular Structure</i> , 2017, 1150, 447-458.	3.6	17
409	Modeling σ -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?. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4841-4853.	5.3	5
410	A Computational Study on the Stability of Oxaphosphirane Rings towards Closed-Shell Valence Isomerization. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 2707-2712.	2.0	6
411	Catalytic and Enantioselective Diels-Alder Reactions of (E)-4-Oxopent-2-enoates. <i>Organic Letters</i> , 2017, 19, 3986-3989.	4.6	17
412	A general intermolecular force field based on tight-binding quantum chemical calculations. <i>Journal of Chemical Physics</i> , 2017, 147, 161708.	3.0	53
413	Benchmarking density functional tight binding models for barrier heights and reaction energetics of organic molecules. <i>Journal of Computational Chemistry</i> , 2017, 38, 2171-2185.	3.3	39
414	Assessment of Density Functionals for Computing Thermodynamic Properties of Lanthanide Complexes. <i>ChemPhysChem</i> , 2017, 18, 2688-2696.	2.1	25
415	W4-17: A diverse and high-confidence dataset of atomization energies for benchmarking high-level electronic structure methods. <i>Journal of Computational Chemistry</i> , 2017, 38, 2063-2075.	3.3	120

#	ARTICLE	IF	CITATIONS
416	Accurate DFT-D3 Calculations in a Small Basis Set. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3575-3585.	5.3	70
417	Dynamic covalent bond from first principles: Diarylbibenzofuranone structural, electronic, and oxidation studies. <i>Journal of Computational Chemistry</i> , 2017, 38, 2675-2679.	3.3	3
418	Bias-Free Chemically Diverse Test Sets from Machine Learning. <i>ACS Combinatorial Science</i> , 2017, 19, 544-554.	3.8	10
419	Ultra-high cycling stability of poly(vinylphenothiazine) as a battery cathode material resulting from π - π interactions. <i>Energy and Environmental Science</i> , 2017, 10, 2334-2341.	30.8	194
420	Quantenchemische Methoden im Leistungsvergleich: Stimmt die Richtung noch?. <i>Angewandte Chemie</i> , 2017, 129, 11155-11163.	2.0	14
421	Time-Dependent Double-Hybrid Density Functionals with Spin-Component and Spin-Opposite Scaling. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4307-4323.	5.3	60
422	Evaluation of the hydrogen adsorption onto Li and Li ⁺ decorated circumtrindene (C ₃₆ H ₁₂): A theoretical study. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 22973-22986.	7.1	14
423	Comparative Computational Study on the Reaction of Chloroacetone with Trimethylphosphite: Perkow versus Michaelis-Arbuzov Reaction Paths. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6517-6522.	2.5	12
424	Performance of a nonempirical exchange functional from density matrix expansion: comparative study with different correlations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21707-21713.	2.8	20
425	Best methods for calculating interaction energies in 2-butene and butane systems. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 150-161.	2.5	3
426	A Combined Theoretical and FT-IR Spectroscopy Study of a Hybrid Poly(furfuryl alcohol) - Lignin Material: Basic Chemistry of a Sustainable Wood Protection Method.. <i>ChemistrySelect</i> , 2017, 2, 10818-10827.	1.5	18
427	Vibrational Structure in Magnetic Circular Dichroism Spectra of Polycyclic Aromatic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9064-9073.	2.5	11
428	Lennard-Jones Potentials for the Interaction of CO ₂ with Five-Membered Aromatic Heterocycles. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9518-9530.	2.5	7
429	Kinetics of the CH ₃ + C ₅ H ₅ Reaction: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9191-9200.	2.5	27
430	Heats of Formation of Medium-Sized Organic Compounds from Contemporary Electronic Structure Methods. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3537-3560.	5.3	45
431	New quantum chemical computations of formamide deuteration support gas-phase formation of this prebiotic molecule. <i>Monthly Notices of the Royal Astronomical Society: Letters</i> , 2017, 468, L1-L5.	3.3	45
432	On the opposite-spin to same-spin ratio of absolute and interaction MP2 correlation energy in parameter-free spin-opposite-scaled double hybrids. <i>Chemical Physics Letters</i> , 2017, 684, 423-426.	2.6	11
433	The preference for dual-gold(σ) catalysis in the hydro(alkoxylation vs. phenoxylation) of alkynes. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 6416-6425.	2.8	18

#	ARTICLE	IF	CITATIONS
434	Dispersion corrections applied to the TCA family of exchange-correlation functionals. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	4
435	Mechanism of the Copper/TEMPO-Catalyzed Aerobic Oxidation of Alcohols. Chemistry - A European Journal, 2017, 23, 1368-1378.	3.3	45
436	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.	3.3	43
437	Stability of the chlorinated derivatives of the DNA/RNA nucleobases, purine and pyrimidine toward radical formation via homolytic C-Cl bond dissociation. International Journal of Quantum Chemistry, 2017, 117, e25319.	2.0	8
438	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 singlet-triplet gaps. Chemical Physics, 2017, 482, 319-338.	1.9	44
439	Quantum Chemical Approach for Determining Degradation Pathways of Phenol by Electrical Discharge Plasmas. Plasma Chemistry and Plasma Processing, 2017, 37, 5-28.	2.4	7
440	What Factors Control the Reactivity of Cobalt-Imido Complexes in C-H Bond Activation via Hydrogen Abstraction?. ACS Catalysis, 2017, 7, 285-292.	11.2	14
441	Understanding the influence of low-frequency vibrations on the hydrogen bonds of acetic acid and acetamide dimers. Physical Chemistry Chemical Physics, 2017, 19, 24866-24878.	2.8	10
442	A Comprehensive Overview of the DFT-D3 London-Dispersion Correction. , 2017, , 195-219.		57
443	Noncovalent Interactions in the Catechol Dimer. Biomimetics, 2017, 2, 18.	3.3	17
444	Synthesis, Crystal Structure, and DFT Study of Ethyl 1-(2-(Hydroxyimino)-2-phenylethyl)-3-phenyl-1H-pyrazole-5-carboxylate. Journal of Chemistry, 2017, 2017, 1-9.	1.9	4
445	Intermolecular Interaction Energies from Kohn-Sham Random Phase Approximation Correlation Methods. , 2017, , 65-136.		6
446	A meta-GGA level screened range-separated hybrid functional by employing short range Hartree-Fock with a long range semilocal functional. Physical Chemistry Chemical Physics, 2018, 20, 8999-9005.	2.8	21
447	FTIR matrix isolation and theoretical studies of glycolic acid dimers. Journal of Molecular Structure, 2018, 1163, 294-299.	3.6	11
448	General Approach To Compute Phosphorescent OLED Efficiency. Journal of Physical Chemistry C, 2018, 122, 6340-6347.	3.1	70
449	Combining covalent bonding and electrostatic attraction to achieve highly viable species with ultrashort beryllium-beryllium distances: a computational design. Dalton Transactions, 2018, 47, 4707-4713.	3.3	16
450	Simplified DFT methods for consistent structures and energies of large systems. Journal of Physics Condensed Matter, 2018, 30, 213001.	1.8	42
451	Advances in modeling hydrocarbon cracking kinetic predictions by quantum chemical theory: A review. International Journal of Energy Research, 2018, 42, 3164-3181.	4.5	11

#	ARTICLE	IF	CITATIONS
452	Linkage Photoisomerization of an Isolated Ruthenium Sulfoxide Complex: Sequential versus Concerted Rearrangement. <i>Inorganic Chemistry</i> , 2018, 57, 5701-5706.	4.0	7
453	Selective ethylene oligomerization with <i>in situ</i> -generated chromium catalysts supported by trifluoromethyl-containing ligands. <i>Journal of Polymer Science Part A</i> , 2018, 56, 444-450.	2.3	3
454	Statistical Analysis of Semiclassical Dispersion Corrections. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2480-2494.	5.3	25
455	Pressure-dependent branching in initial decomposition of gamma-valerolactone: a quantum chemical/RRKM study. <i>RSC Advances</i> , 2018, 8, 12975-12983.	3.6	8
456	High temperature pyrolysis of 2-methyl furan. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10826-10837.	2.8	17
457	B97-3c: A revised low-cost variant of the B97-D density functional method. <i>Journal of Chemical Physics</i> , 2018, 148, 064104.	3.0	400
458	Communication: An improved linear scaling perturbative triples correction for the domain based local pair-natural orbital based singles and doubles coupled cluster method [DLPNO-CCSD(T)]. <i>Journal of Chemical Physics</i> , 2018, 148, 011101.	3.0	402
459	Performance of Density Functional Theory for Predicting Methane-to-Methanol Conversion by a Tri-Copper Complex. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1024-1036.	3.1	23
460	Parametrization and Benchmark of Long-Range Corrected DFTB2 for Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 115-125.	5.3	60
461	Accelerating the coupled-cluster singles and doubles method using the chain-of-sphere approximation. <i>Molecular Physics</i> , 2018, 116, 1428-1434.	1.7	19
462	Rational Density Functional Selection Using Game Theory. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 61-67.	5.4	20
463	rPM6 parameters for phosphorous and sulphur-containing open-shell molecules. <i>Molecular Physics</i> , 2018, 116, 602-610.	1.7	2
464	Homogeneously Catalyzed Electroreduction of Carbon Dioxide—Methods, Mechanisms, and Catalysts. <i>Chemical Reviews</i> , 2018, 118, 4631-4701.	47.7	858
465	A molecular electron density theory study of the chemo- and regioselective [3+2] cycloaddition reactions between trifluoroacetonitrile N-oxide and thioketones. <i>Chemical Physics</i> , 2018, 501, 128-137.	1.9	11
466	Disulfuryl Dichloride ClSO ₂ OSO ₂ Cl: A Conformation and Polymorphism Chameleon. <i>Chemistry - A European Journal</i> , 2018, 24, 10409-10421.	3.3	4
467	Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates III: Butylbenzene Isomers (<i>n</i> -, <i>s</i> -, and <i>t</i> -C ₁₄ H ₁₀). <i>Journal of Physical Chemistry A</i> , 2018, 122, 3980-4001.	2.5	16
468	Thermodynamic and kinetic hydricities of metal-free hydrides. <i>Chemical Society Reviews</i> , 2018, 47, 2809-2836.	38.1	103
469	Identifying intermediates in the reductive intramolecular cyclisation of allyl 2-bromobenzyl ether by an improved electron paramagnetic resonance spectroelectrochemical electrode design combined with density functional theory calculations. <i>Electrochimica Acta</i> , 2018, 271, 10-18.	5.2	10

#	ARTICLE	IF	CITATIONS
470	How Accurate Is Density Functional Theory at Predicting Dipole Moments? An Assessment Using a New Database of 200 Benchmark Values. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1969-1981.	5.3	180
471	Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection. <i>Astrophysical Journal</i> , 2018, 855, 123.	4.5	35
472	The Genealogical Tree of Ethanol: Gas-phase Formation of Glycolaldehyde, Acetic Acid, and Formic Acid. <i>Astrophysical Journal</i> , 2018, 854, 135.	4.5	103
473	Long-range corrected density functional through the density matrix expansion based semilocal exchange hole. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8991-8998.	2.8	21
474	The hows and whys of peculiar coordination of 4-amino-2,1,3-benzothiadiazole. <i>Polyhedron</i> , 2018, 139, 33-43.	2.2	16
475	Analysis of the conformational properties of amine ligands at the gold/water interface with QM, MM and QM/MM simulations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3349-3362.	2.8	15
476	Computerchemie: das Schicksal aktueller Methoden und zukünftige Herausforderungen. <i>Angewandte Chemie</i> , 2018, 130, 4241-4248.	2.0	16
477	Computational Chemistry: The Fate of Current Methods and Future Challenges. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 4170-4176.	13.8	138
478	Benchmarking of DFT functionals for the kinetics and mechanisms of atmospheric addition reactions of OH radicals with phenyl and substituted phenyl-based organic pollutants. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25533.	2.0	14
479	Quantitative Assessment of rPM6 for Fluorine- and Chlorine-Containing Metal Complexes: Comparison with Experimental, First-Principles, and Other Semiempirical Results. <i>Molecules</i> , 2018, 23, 3332.	3.8	1
480	â€ˆDiet GMTKN55â€™ offers accelerated benchmarking through a representative subset approach. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27735-27739.	2.8	26
481	Stabilization of beryllium-containing planar pentacoordinate carbon species through attaching hydrogen atoms. <i>RSC Advances</i> , 2018, 8, 36521-36526.	3.6	20
482	Preparation and Properties of Chlorosulfonyl Chloroformate, ClC(O)OSO ₂ Cl. <i>Inorganic Chemistry</i> , 2018, 57, 14834-14842.	4.0	1
483	Electronic spectroscopy of methyl vinyl ketone oxide: A four-carbon unsaturated Criegee intermediate from isoprene ozonolysis. <i>Journal of Chemical Physics</i> , 2018, 149, 244309.	3.0	44
484	Quantum Chemical Calculations on CHOP Derivativesâ€™ Spanning the Chemical Space of Phosphinidenes, Phosphaketenes, Oxaphosphirenes, and COPâ€™ Isomers. <i>Molecules</i> , 2018, 23, 3341.	3.8	13
485	Communication: Strong-interaction limit of an adiabatic connection in Hartree-Fock theory. <i>Journal of Chemical Physics</i> , 2018, 149, 241101.	3.0	25
486	Potential of quantum computing for drug discovery. <i>IBM Journal of Research and Development</i> , 2018, 62, 6:1-6:20.	3.1	130
487	Roaming-like Mechanism for Dehydration of Diol Radicals. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9738-9754.	2.5	7

#	ARTICLE	IF	CITATIONS
488	Intermolecular dissociation energies of hydrogen-bonded 1-naphthol complexes. Journal of Chemical Physics, 2018, 149, 204311.	3.0	8
489	Isomerism of the Aniline Trimer. Angewandte Chemie, 2018, 130, 15332-15336.	2.0	6
490	Orientation of AgI Ions in Coordination Architectures through Ligand Conformation and Anion Binding: from Polymeric Chains to Discrete Squares. European Journal of Inorganic Chemistry, 2018, 2018, 4278-4285.	2.0	1
491	Molecular insight into the interaction mechanisms of an annulated pyrazole (DB08446) with HIV-1 RT: a QM and QM/QM study. Monatshefte für Chemie, 2018, 149, 1919-1929.	1.8	1
492	Dependence of Heterogeneous Nucleation on Hydrogen Bonding Lifetime and Complementarity. Crystal Growth and Design, 2018, 18, 7158-7172.	3.0	19
493	Isomerism of the Aniline Trimer. Angewandte Chemie - International Edition, 2018, 57, 15112-15116.	13.8	19
494	Systematic High-Accuracy Prediction of Electron Affinities for Biological Quinones. Journal of Computational Chemistry, 2018, 39, 2439-2451.	3.3	9
495	A Simple Correction for Nonadditive Dispersion within Extended Symmetry-Adapted Perturbation Theory (XSAPT). Journal of Chemical Theory and Computation, 2018, 14, 5128-5142.	5.3	19
496	The Nonlocal Kernel in van der Waals Density Functionals as an Additive Correction: An Extensive Analysis with Special Emphasis on the B97M-V and PBE0-B97M-V Approaches. Journal of Chemical Theory and Computation, 2018, 14, 5725-5738.	5.3	170
497	Fermi-Dirac in orbital self-interaction corrected density functional theory: Ionization potentials and enthalpies of formation. Journal of Computational Chemistry, 2018, 39, 2463-2471.	3.3	35
498	Performance of density functional theory for describing hetero-metallic active-site motifs for methane-to-methanol conversion in metal-exchanged zeolites. Journal of Computational Chemistry, 2018, 39, 2667-2678.	3.3	8
499	London Dispersion Interactions in Pnictogen Cations [ECI ₂] ⁺ and [E=E] ²⁺ (E=P, As, Sb) Supported by Anionic <i>N</i> -Heterocyclic Carbenes. Chemistry - A European Journal, 2018, 24, 18922-18932.	3.3	47
500	Quantum chemistry reveals thermodynamic principles of redox biochemistry. PLoS Computational Biology, 2018, 14, e1006471.	3.2	22
501	Exploiting the Ring Strain of Diphosphetanes: A Synthetic and Computational Approach towards 1,2,5-selenadiphospholanes. ChemPlusChem, 2018, 83, 1057-1064.	2.8	7
502	Facial and Meridional Isomers of Tris(bidentate) Ir(III) Complexes: Unravelling Their Different Excited State Reactivity. Inorganic Chemistry, 2018, 57, 12106-12112.	4.0	38
503	Error-Controlled Exploration of Chemical Reaction Networks with Gaussian Processes. Journal of Chemical Theory and Computation, 2018, 14, 5238-5248.	5.3	62
504	Reduktion von Phosphanoxiden mit Oxalylchlorid und Wasserstoff, vermittelt durch ein elektrophiles Phosphoniumkation. Angewandte Chemie, 2018, 130, 15473-15476.	2.0	7
505	Electrophilic Phosphonium Cation-Mediated Phosphane Oxide Reduction Using Oxalyl Chloride and Hydrogen. Angewandte Chemie - International Edition, 2018, 57, 15253-15256.	13.8	37

#	ARTICLE	IF	CITATIONS
506	Exploring conformational preferences of alanine tetrapeptide by CCSD(T), MP2, and dispersion-corrected DFT methods. <i>Chemical Physics Letters</i> , 2018, 702, 69-75.	2.6	12
507	Restoring Size Consistency of Approximate Functionals Constructed from the Adiabatic Connection. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3137-3142.	4.6	26
508	A Comprehensive Assessment of the Effectiveness of Orbital Optimization in Double-Hybrid Density Functionals in the Treatment of Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5610-5624.	2.5	19
509	The theoretical chemical calculations clarify the mechanism of beta-alkylation of 1-phenylethanol with benzyl alcohol catalyzed by iron(II) acetylacetonate methods. <i>RSC Advances</i> , 2018, 8, 24154-24165.	3.6	1
510	Wavefunction-like Correlation Model for Use in Hybrid Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4590-4599.	5.3	3
511	Semi-empirical or non-empirical double-hybrid density functionals: which are more robust?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23175-23194.	2.8	102
512	Combining Wave Function Methods with Density Functional Theory for Excited States. <i>Chemical Reviews</i> , 2018, 118, 7249-7292.	47.7	166
513	Communication: Accurate description of interaction energies and three-body effects in weakly bound molecular complexes by PBE-QIDH models. <i>Journal of Chemical Physics</i> , 2018, 149, 041101.	3.0	4
514	Efficient and Accurate Prediction of Nuclear Magnetic Resonance Shielding Tensors with Double-Hybrid Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4756-4771.	5.3	75
515	Four-Carbon Criegee Intermediate from Isoprene Ozonolysis: Methyl Vinyl Ketone Oxide Synthesis, Infrared Spectrum, and OH Production. <i>Journal of the American Chemical Society</i> , 2018, 140, 10866-10880.	13.7	109
516	Assessing the performance of the Tao-Mo semilocal density functional in the projector-augmented-wave method. <i>Journal of Chemical Physics</i> , 2018, 149, 044120.	3.0	50
517	Strategy Used for Controlling the Photostability of Tridentate Pt(II) Complexes To Enhance the Device Lifetimes of Blue Phosphorescent Organic Light-Emitting Diodes: The Role of the Pt-C*(NHC) Bond and Auxiliary Ligand. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16872-16878.	3.1	6
518	How accurate are static polarizability predictions from density functional theory? An assessment over 132 species at equilibrium geometry. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19800-19810.	2.8	94
519	On the Mechanism of Trimethylphosphine-Mediated Reductive Dimerization of Ketones. <i>Inorganic Chemistry</i> , 2018, 57, 8058-8064.	4.0	18
520	Computational modelling of singlet excitation energy transfer: a DFT/TD-DFT study of the ground and excited state properties of a syn bimane dimer system using non-empirically tuned range-separated functionals. <i>New Journal of Chemistry</i> , 2018, 42, 13732-13743.	2.8	2
521	MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling. , 2018, , 1-21.		1
522	Accurate theoretical method for homolytic cleavage of C Sn bond: A benchmark approach. <i>Computational and Theoretical Chemistry</i> , 2018, 1140, 134-144.	2.5	11
523	Accurate Spin-State Energetics for Aryl Carbenes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4733-4746.	5.3	25

#	ARTICLE	IF	CITATIONS
524	Predicting vapor liquid equilibria using density functional theory: A case study of argon. Journal of Chemical Physics, 2018, 148, 224501.	3.0	10
525	Survival of the most transferable at the top of Jacob's ladder: Defining and testing the B97M(2) double hybrid density functional. Journal of Chemical Physics, 2018, 148, 241736.	3.0	136
526	Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1378.	14.6	95
527	Statistically representative databases for density functional theory via data science. Physical Chemistry Chemical Physics, 2019, 21, 19092-19103.	2.8	20
528	Efficient band gap prediction of semiconductors and insulators from a semilocal exchange-correlation functional. Physical Review B, 2019, 100, .	3.2	35
529	Toward a Quantum-Chemical Benchmark Set for Enzymatically Catalyzed Reactions: Important Steps and Insights. Journal of Physical Chemistry A, 2019, 123, 7057-7074.	2.5	19
530	Cost-effective density functional theory (DFT) calculations of equilibrium isotopic fractionation in large organic molecules. Physical Chemistry Chemical Physics, 2019, 21, 17555-17570.	2.8	11
531	B2PLYP and B2GPPLYP: The First Two Double-Hybrid Density Functionals with Long-Range Correction Optimized for Excitation Energies. Journal of Chemical Theory and Computation, 2019, 15, 4735-4744.	5.3	107
532	Accurate Binding Energies for Lithium Polysulfides and Assessment of Density Functionals for Lithium-Sulfur Battery Research. Journal of Physical Chemistry C, 2019, 123, 20737-20747.	3.1	34
533	Dibenzo-p-dioxin. Twisted and puckered excited state molecular geometries. Computational and Theoretical Chemistry, 2019, 1164, 112551.	2.5	1
534	Preparation, characterization, in vitro and in vivo evaluation of metronidazole-gallic acid cocrystal: A combined experimental and theoretical investigation. Journal of Molecular Structure, 2019, 1197, 727-735.	3.6	17
535	Combined Density Functional and Algebraic-Diagrammatic Construction Approach for Accurate Excitation Energies and Transition Moments. Journal of Chemical Theory and Computation, 2019, 15, 4440-4453.	5.3	21
536	Self-Assemble and In Situ Formation of Laponite RDS Decorated Ti ₃ C ₂ T _x Hybrids for Application in Lithium-Ion Battery. ChemistrySelect, 2019, 4, 10694-10700.	1.5	5
537	Data-Driven Materials Science: Status, Challenges, and Perspectives. Advanced Science, 2019, 6, 1900808.	11.2	358
538	Geometric E ⁺ Z Isomerisation of Alkenyl Silanes by Selective Energy Transfer Catalysis: Stereodivergent Synthesis of Triarylethylenes via a Formal anti-Metallometallation. Angewandte Chemie - International Edition, 2019, 58, 18619-18626.	13.8	52
539	PEPCONF, a diverse data set of peptide conformational energies. Scientific Data, 2019, 6, 180310.	5.3	23
540	Construction of a Range-Separated Dual-Hybrid Direct Random Phase Approximation. Journal of Chemical Theory and Computation, 2019, 15, 6678-6687.	5.3	10
541	Geometric E ⁺ Z Isomerisation of Alkenyl Silanes by Selective Energy Transfer Catalysis: Stereodivergent Synthesis of Triarylethylenes via a Formal anti-Metallometallation. Angewandte Chemie, 2019, 131, 18792-18799.	2.0	16

#	ARTICLE	IF	CITATIONS
542	Stability of σ -No-Pair Ferromagnetic Lithium Clusters. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9721-9728.	2.5	3
543	Exploring Nature and Predicting Strength of Hydrogen Bonds: A Correlation Analysis Between Atoms-Molecules Descriptors, Binding Energies, and Energy Components of Symmetry-Adapted Perturbation Theory. <i>Journal of Computational Chemistry</i> , 2019, 40, 2868-2881.	3.3	678
544	Hydrogen Atom Transfer Induced Boron Retaining Coupling of Organoboronic Esters and Organolithium Reagents. <i>Journal of the American Chemical Society</i> , 2019, 141, 14126-14130.	13.7	51
545	Copper hydride-mediated electrophilic amidation of vinylarenes with dioxazolones – a computational mechanistic study. <i>Dalton Transactions</i> , 2019, 48, 14337-14346.	3.3	4
546	Soft experimental constraints for soft interactions: a spectroscopic benchmark data set for weak and strong hydrogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18799-18810.	2.8	20
547	Screened hybrid meta-GGA exchange-correlation functionals for extended systems. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3002-3015.	2.8	16
548	Influence of chelate ring type on chelate-chelate and chelate-aryl stacking: the case of nickel bis(dithiolene). <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1198-1206.	2.8	7
549	TEMPO-Mediated Catalysis of the Sterically Hindered Hydrogen Atom Transfer Reaction between $(C_5H_5)_5Cr(CO)_3H$ and a Trityl Radical. <i>Journal of the American Chemical Society</i> , 2019, 141, 1882-1886.	13.7	25
550	The impact on the ring related vibrational frequencies of pyridine of hydrogen bonds with haloforms – a topology perspective. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1724-1736.	2.8	12
551	Face, Notch, or Edge? Intermolecular dissociation energies of 1-naphthol complexes with linear molecules. <i>Journal of Chemical Physics</i> , 2019, 150, 234303.	3.0	10
552	Improving the Performance of Tao's Mo Non-empirical Density Functional with Broader Applicability in Quantum Chemistry and Materials Science. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6356-6369.	2.5	29
553	A microwave spectroscopic and <i>ab initio</i> study of keto-enol tautomerism and isomerism in the cyclohexanone-water complex. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12872-12880.	2.8	10
554	Minimally Empirical Double-Hybrid Functionals Trained against the GMTKN55 Database: revDSD-PBEP86-D4, revDOD-PBE-D4, and DOD-SCAN-D4. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5129-5143.	2.5	262
555	Potential-Energy Surfaces for Ring-Puckering Motions of Flexible Cyclic Molecules through Cremer-Pople Coordinates: Computation, Analysis, and Fitting. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4280-4294.	5.3	23
556	PyFrag 2019 – Automating the exploration and analysis of reaction mechanisms. <i>Journal of Computational Chemistry</i> , 2019, 40, 2227-2233.	3.3	57
557	Performance of new density functionals of nondynamic correlation on chemical properties. <i>Journal of Chemical Physics</i> , 2019, 150, 204101.	3.0	9
558	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. <i>Chemical Reviews</i> , 2019, 119, 8131-8191.	47.7	167
559	Gas-Phase Synthesis and Reactivity of Ligated Group 10 Ions in the Formal +1 Oxidation State. <i>Journal of the American Society for Mass Spectrometry</i> , 2019, 30, 1867-1880.	2.8	7

#	ARTICLE	IF	CITATIONS
560	Adsorption behavior of mercuric oxide clusters on activated carbon and the effect of SO ₂ on this adsorption: a theoretical investigation. <i>Journal of Molecular Modeling</i> , 2019, 25, 142.	1.8	18
561	Accessing the First <i>nido</i> -Carborane-Substituted Diphosphetane: A Ligand and Synthon for <i>nido</i> -Carboranylphosphanes. <i>Chemistry - A European Journal</i> , 2019, 25, 11456-11465.	3.3	7
562	Design of stable platinum(II) complexes exhibited various colors via auxiliary ligand and electron-donating/withdrawing groups: A theoretical investigation. <i>Organic Electronics</i> , 2019, 71, 251-257.	2.6	4
563	Assessment of Double-Hybrid Density Functional Theory for Magnetic Exchange Coupling in Manganese Complexes. <i>Inorganics</i> , 2019, 7, 57.	2.7	19
564	Oxidation energies of shuttle molecules candidates in lithium-ion batteries from double-hybrid models. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25950.	2.0	7
565	<i>Mer</i> - <i>Cr</i> (ppy) ₃ to <i>Fac</i> - <i>Cr</i> (ppy) ₃ Photoisomerization. <i>ChemPhotoChem</i> , 2019, 3, 697-701.	3.0	11
566	Methane activation by alternant [N ₂ O ₂] ⁺ and [N ₂ S ₂] ⁺ cluster radical cations. <i>International Journal of Mass Spectrometry</i> , 2019, 438, 72-77.	1.5	0
567	Mechanistic study on iron(II)-mediated direct arylation of benzene with chlorobenzene. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25912.	2.0	1
568	On a specific state of C ₆₀ fullerene in N-methyl-2-pyrrolidone solution: Mass spectrometric study. <i>Applied Surface Science</i> , 2019, 481, 1566-1572.	6.1	12
569	Well-behaved versus ill-behaved density functionals for single bond dissociation: Separating success from disaster functional by functional for stretched H ₂ . <i>Journal of Chemical Physics</i> , 2019, 150, 094115.	3.0	25
570	DFT study on selective autocatalyzed $\text{C}_{10}\text{H}_8\text{O}_2$ -alkylation of ketones with alcohols. <i>Journal of Catalysis</i> , 2019, 373, 126-138.	6.2	6
571	Main-group test set for materials science and engineering with user-friendly graphical tools for error analysis: systematic benchmark of the numerical and intrinsic errors in state-of-the-art electronic-structure approximations. <i>New Journal of Physics</i> , 2019, 21, 013025.	2.9	15
572	The Lowest-Energy Isomer of C ₂ Si ₂ H ₄ Is a Bridged Ring: Reinterpretation of the Spectroscopic Data Based on DFT and Coupled-Cluster Calculations. <i>Inorganics</i> , 2019, 7, 51.	2.7	0
573	Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchange-Correlation Functionals: The MOBH35 Benchmark Database. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3761-3781.	2.5	104
574	Hydrodynamic volume of trehalose and its water uptake mechanism. <i>Biophysical Chemistry</i> , 2019, 249, 106145.	2.8	4
575	Copper(<i>scp</i>)-catalyzed asymmetric aza Diels-Alder reactions of azoalkenes toward fulvenes: a molecular electron density theory study. <i>New Journal of Chemistry</i> , 2019, 43, 4765-4776.	2.8	21
576	Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1743-1760.	5.3	45
577	Organic Compounds of Actinyls: Systematic Computational Assessment of Structural and Topological Properties in [AnO ₂](C ₂ O ₄) ₃ ·nH ₂ O (An = Th, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr). <i>Inorganic Chemistry</i> , 2019, 58, 1174-1184.	4.0	11

#	ARTICLE	IF	CITATIONS
578	A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User. Australian Journal of Chemistry, 2019, 72, 563.	0.9	115
579	Conversion mechanism and isomeric preferences of the cis and trans isomers of anti-cancer medicine carmustine; A double hybrid DFT calculation. Chemical Physics, 2019, 522, 39-43.	1.9	6
580	Dispersion-driven conformational preference in the gas phase: Microwave spectroscopic and theoretical study of allyl isocyanate. Journal of Chemical Physics, 2019, 151, 194304.	3.0	6
581	Catalytic Hydrolysis Mechanism of Cocaine by Human Carboxylesterase 1: An Orthoester Intermediate Slows Down the Reaction. Molecules, 2019, 24, 4057.	3.8	3
582	Asymmetric Total Synthesis of (âˆ“)Pavidolide B via a Thiyl-Radical-Mediated [3 + 2] Annulation Reaction. Journal of Organic Chemistry, 2019, 84, 15958-15971.	3.2	14
583	Actinide Endohedral and Exohedral Cubic Siloxanes: An(IV)@ (HSiO_{1.5})₈ and An(IV)&(RSiO_{1.5})₈ (An = U, Np, Pu; R = H, Cl, OH). European Journal of Inorganic Chemistry, 2019, 2019, 4660-4667.	2.0	2
584	ACCCDB: A collection of chemistry databases for broad computational purposes. Journal of Computational Chemistry, 2019, 40, 839-848.	3.3	42
585	Exploring density functional subspaces with genetic algorithms. Monatshefte FÃ¼r Chemie, 2019, 150, 173-182.	1.8	8
586	Evaluating Density Functionals by Examining Molecular Structures, Chemical Bonding, and Relative Energies of Mononuclear Ruâ€“Clâ€“Hâ€“PR ₃ Isomers. Journal of Physical Chemistry A, 2019, 123, 343-358.	2.5	1
587	Hydrogen-Bond-Dependent Conformational Switching: A Computational Challenge from Experimental Thermochemistry. Journal of Organic Chemistry, 2019, 84, 613-621.	3.2	5
588	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.	2.5	13
589	Unprecedented Mechanism of an Organocatalytic Route to Conjugated Enynes with a Junction to Cyclic Nitronates. European Journal of Organic Chemistry, 2019, 2019, 328-337.	2.4	7
590	Ligand-Dependent Multi-State Reactivity in Cobalt(III)-Catalyzed Câ€“H Activations. ACS Catalysis, 2019, 9, 1962-1972.	11.2	25
591	Generalized Prediction of Enthalpies of Formation Using DLPNOâ€“CCSD(T) Ab Initio Calculations for Molecules Containing the Elements H, C, N, O, F, S, Cl, Br. Journal of Computational Chemistry, 2019, 40, 768-793.	3.3	15
592	Accurate heats of formation of polycyclic saturated hydrocarbons predicted by using the XYG3 type of doubly hybrid functionals. Journal of Computational Chemistry, 2019, 40, 1113-1122.	3.3	6
593	A comparison of the structure and bonding in the donorâ€“acceptor complexes H ₃ N â†’ BR(OH) ₂ and H ₃ N â†’ BRH(OH) (R = H; NH ₂ , OH, and F): a computational investigation. Structural Chemistry, 2019, 30, 361-368.	2.0	3
594	Mechanism and rate constants of the CH ₂ + CH ₂ CO reactions in triplet and singlet states: A theoretical study. Journal of Computational Chemistry, 2019, 40, 387-399.	3.3	12
595	Performance of DFT for C₆₀ Isomerization Energies: A Noticeable Exception to Jacobâ€™s Ladder. Journal of Physical Chemistry A, 2019, 123, 257-266.	2.5	19

#	ARTICLE	IF	CITATIONS
596	Does the gradient-regulated connection improve the description of correlated metal bond properties?. International Journal of Quantum Chemistry, 2019, 119, e25831.	2.0	0
597	Investigations of Stacked DNA Base-Pair Steps: Highly Accurate Stacking Interaction Energies, Energy Decomposition, and Many-Body Stacking Effects. Journal of Chemical Theory and Computation, 2019, 15, 95-115.	5.3	55
598	The Taming of Redox-Labile Phosphidotitanocene Cations. Chemistry - A European Journal, 2019, 25, 2803-2815.	3.3	11
599	Impact of the \pm -Ferrocenyl Group on the Solvolytic Reactivity - Electrofugality - of Ferrocenylphenylmethyl Cations. European Journal of Organic Chemistry, 2019, 2019, 537-546.	2.4	4
600	Photophysical insights and guidelines for blue π -conjugated fluorescent probes for the direct detection of nitric oxide (NO) in biological systems. Journal of Physical Organic Chemistry, 2019, 32, e3896.	1.9	5
601	How does SCAN compare to PBE in the framework of parameter-free spin-opposite-scaled double-hybrids?. Chemical Physics Letters, 2020, 738, 136898.	2.6	5
602	Electronic spectroscopic characterization of the formation of iron(III) metal complexes: The 8-HydroxyQuinoline as ligand case study. Journal of Inorganic Biochemistry, 2020, 203, 110864.	3.5	11
603	A Triazole-Substituted Aryl Iodide with Omnipotent Reactivity in Enantioselective Oxidations. Angewandte Chemie, 2020, 132, 1495-1500.	2.0	15
604	A Triazole-Substituted Aryl Iodide with Omnipotent Reactivity in Enantioselective Oxidations. Angewandte Chemie - International Edition, 2020, 59, 1479-1484.	13.8	65
605	Understanding chemical reactivity using the activation strain model. Nature Protocols, 2020, 15, 649-667.	12.0	188
606	Unravelling the mechanism of cobalt-catalysed remote C-H nitration of 8-aminoquinolinamides and expansion of substrate scope towards 1-naphthylpicolinamide. Chemical Science, 2020, 11, 534-542.	7.4	1
607	Accuracy of semiexperimental equilibrium structures: Sulfine as an example. Journal of Molecular Structure, 2020, 1206, 127676.	3.6	9
608	Accurate Water Properties from an Efficient ab Initio Method. Journal of Chemical Theory and Computation, 2020, 16, 974-987.	5.3	15
609	Fluxional nature in cyclohexane and cyclopentane: spherical conformational landscape model revisited. Journal of Chemical Sciences, 2020, 132, 1.	1.5	4
610	Benchmark study of DFT and composite methods for bond dissociation energies in argon compounds. Chemical Physics, 2020, 531, 110676.	1.9	8
611	Empirical Double-Hybrid Density Functional Theory: A "Third Way" in Between WFT and DFT. Israel Journal of Chemistry, 2020, 60, 787-804.	2.3	129
612	Comprehensive Benchmark Results for the Domain Based Local Pair Natural Orbital Coupled Cluster Method (DLPNO-CCSD(T)) for Closed- and Open-Shell Systems. Journal of Physical Chemistry A, 2020, 124, 90-100.	2.5	169
613	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.	3.3	13

#	ARTICLE	IF	CITATIONS
614	Effect of molecular backbone structure on vapor phase coupling reaction between diiso(thio)cyanates with diamines, diols, and dithiols. <i>Progress in Organic Coatings</i> , 2020, 140, 105509.	3.9	4
615	Conformational preferences of cationic $\hat{\text{I}}^2$ -peptide in water studied by CCSD(T), MP2, and DFT methods. <i>Heliyon</i> , 2020, 6, e04721.	3.2	4
616	Comparison of Vitamin C and Its Derivative Antioxidant Activity: Evaluated by Using Density Functional Theory. <i>ACS Omega</i> , 2020, 5, 25467-25475.	3.5	38
617	Infrared Spectra of (<i>Z</i>)- and (<i>E</i>)- $\text{C}_{2\text{H}_3\text{C}(\text{CH}_3)_2\text{I}}$ Radicals Produced upon Photodissociation of (<i>Z</i>)- and (<i>E</i>)- $(\text{CH}_2)_2\text{HC}\cdot\text{C}(\text{CH}_3)_2\text{I}$ in Solid <i>para</i> -Hydrogen. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5887-5895.	2.5	3
618	Synthesis, X-ray structures and magnetic properties of Ni(II) complexes of heteroaromatic hydrazone. <i>Polyhedron</i> , 2020, 191, 114802.	2.2	5
619	Unsupervised search of low-lying conformers with spectroscopic accuracy: A two-step algorithm rooted into the island model evolutionary algorithm. <i>Journal of Chemical Physics</i> , 2020, 153, 124110.	3.0	30
620	A Local Hybrid Functional with Wide Applicability and Good Balance between (De)Localization and Left-Right Correlation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5645-5657.	5.3	54
621	Formation of Phenanthrene via Recombination of Indenyl and Cyclopentadienyl Radicals: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9933-9941.	2.5	17
622	A chemical dynamics study on the gas-phase formation of triplet and singlet C_{5H_2} carbenes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 30142-30150.	7.1	16
623	Influence of solvent on crystal nucleation of benzocaine. <i>CrystEngComm</i> , 2020, 22, 8330-8342.	2.6	4
624	Structural isomers of saligenin-based $\hat{\text{I}}^2$ -agonists: synthesis and insight into the reaction mechanism. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 9675-9688.	2.8	2
625	Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7166-7176.	2.5	45
626	Structure, Stability, and Spectroscopic Properties of Small Acetonitrile Cation Clusters. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6845-6855.	2.5	6
627	Atomistic simulations of the aggregation of small aromatic molecules in homogenous and heterogenous mixtures. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21005-21014.	2.8	3
628	Basis Set Extrapolations for Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5712-5722.	5.3	13
629	Full Conformational Analyses of the Ultrafast Isomerization in Penta-coordinated $\text{Ru}(\text{S}_2\text{C}_2(\text{CF}_3)_2)(\text{CO})(\text{PPh}_3)_2$: One Compound, Two Crystal Structures, Three CO Frequencies, 24 Stereoisomers, and 48 Transition States. <i>Inorganic Chemistry</i> , 2020, 59, 11757-11769.	4.0	1
630	DFT Study on the Mechanism of 4,4'-Bipyridine-Catalyzed Nitrobenzene Reduction by Diboron(4) Compounds. <i>Journal of Organic Chemistry</i> , 2020, 85, 13877-13885.	3.2	10
631	The KDEL trafficking receptor exploits pH to tune the strength of an unusual short hydrogen bond. <i>Scientific Reports</i> , 2020, 10, 16903.	3.3	11

#	ARTICLE	IF	CITATIONS
632	Extended Koopmans's TM theorem in the adiabatic connection formalism: Applied to doubly hybrid density functionals. <i>Journal of Chemical Physics</i> , 2020, 153, 044109.	3.0	5
633	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. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22508-22519.	2.8	68
634	One-Step Instantaneous Detection of Multiple Military and Improvised Explosives Facilitated by Colorimetric Reagent Design. <i>Analytical Chemistry</i> , 2020, 92, 13980-13988.	6.5	31
635	Accurate Hybrid Density Functionals with UW12 Correlation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6176-6194.	5.3	5
636	Gas Phase Synthesis of the Elusive Trisilacyclopropyl Radical (Si_3H_5) via Unimolecular Decomposition of Chemically Activated Doublet Trisilapropyl Radicals (Si_3H_7). <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 7874-7881.	4.6	0
637	Assessing the Tamm-Dancoff approximation, singlet-singlet, and singlet-triplet excitations with the latest long-range corrected double-hybrid density functionals. <i>Journal of Chemical Physics</i> , 2020, 153, 064106.	3.0	54
638	Efficient yet accurate dispersion-corrected semilocal exchange-correlation functionals for non-covalent interactions. <i>Journal of Chemical Physics</i> , 2020, 153, 084117.	3.0	10
639	DFT, DLPNO-CCSD(T), and NEVPT2 benchmark study of the reaction between ferrocenium and trimethylphosphine. <i>Journal of Computational Chemistry</i> , 2020, 41, 2388-2397.	3.3	12
640	New theoretical insights into the reaction kinetics of toluene and hydroxyl radicals. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22279-22288.	2.8	11
641	FLP-catalysis meets hydrogen-bond activation. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 7321-7325.	2.8	4
642	Efficient Treatment of Correlation Energies at the Basis-Set Limit by Monte Carlo Summation of Continuum States. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6550-6559.	5.3	2
643	Nature of intermolecular interaction in squaraine dimers. <i>Scientific Reports</i> , 2020, 10, 19670.	3.3	7
644	Actinyl-Carboxylate Complexes $[\text{AnO}_2(\text{COOH})_n(\text{H}_2\text{O})_m]^{2-n-m}$ (An = U, Np, Pu, and Am; $n = 1-3$; $m = 0, 2, 4$; $2n + m = 6$): Electronic Structures, Interaction Features, and the Potential to Adsorb toward Cs Ion. <i>ACS Omega</i> , 2020, 5, 31974-31983.	3.5	2
645	Molecular dynamics simulations of liquid-liquid interfaces in an electric field: The water-1,2-dichloroethane interface. <i>Journal of Chemical Physics</i> , 2020, 153, 164714.	3.0	8
646	The corona of a surface bubble promotes electrochemical reactions. <i>Nature Communications</i> , 2020, 11, 6323.	12.8	72
647	Third-Order Møller-Plesset Theory Made More Useful? The Role of Density Functional Theory Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7473-7489.	5.3	27
648	1,1-Bisborylalkanes via Radical Boron Migration. <i>Journal of the American Chemical Society</i> , 2020, 142, 9119-9123.	13.7	54
649	The one-electron self-interaction error in 74 density functional approximations: a case study on hydrogenic mono- and dinuclear systems. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15805-15830.	2.8	27

#	ARTICLE	IF	CITATIONS
650	Partitioning a Molecule into the Atomic Basins and the Resultant Atomic Charges from Quantum Chemical Topology Analysis of the Kohn–Sham Potential. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5023-5032.	2.5	3
651	MAP: An MP2 Accuracy Predictor for Weak Interactions from Adiabatic Connection Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4141-4149.	5.3	10
652	Prediction of organic homolytic bond dissociation enthalpies at near chemical accuracy with sub-second computational cost. <i>Nature Communications</i> , 2020, 11, 2328.	12.8	128
653	3PO as a Selective Inhibitor of 6-Phosphofructo-2-Kinase/Fructose-2,6-Biphosphatase 3 in A375 Human Melanoma Cells. <i>Anticancer Research</i> , 2020, 40, 2613-2625.	1.1	14
654	Revisiting the Tropospheric OH-Initiated Unimolecular Decomposition of Chlorpyrifos and Chlorpyrifos-Methyl: A Theoretical Perspective. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4280-4289.	2.5	3
655	Theoretical Mechanistic Studies of Rh-Catalyzed C(sp ³)–H Amination: A Comparison with Co Analogue and Metal Effects. <i>Chinese Journal of Chemistry</i> , 2020, 38, 1526-1532.	4.9	4
656	Canonical and DLPNO-Based G4(MP2)XK-Inspired Composite Wave Function Methods Parametrized against Large and Chemically Diverse Training Sets: Are They More Accurate and/or Robust than Double-Hybrid DFT?. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4238-4255.	5.3	30
657	Conformational design concepts for anions in ionic liquids. <i>Chemical Science</i> , 2020, 11, 6405-6422.	7.4	33
658	Selective Quadruple C(sp ³)-F Functionalization of Polyfluoroalkyl Ketones. <i>IScience</i> , 2020, 23, 101259.	4.1	27
659	Density functional theory studies on cytosine analogues for inducing double-proton transfer with guanine. <i>Scientific Reports</i> , 2020, 10, 9671.	3.3	8
660	Remarkable Accuracy of an $\langle i \rangle O \langle /i \rangle (\langle i \rangle N \langle /i \rangle \langle \sup \rangle 6 \langle /sup \rangle)$ Perturbative Correction to Opposite-Spin CCSD: Are Triples Necessary for Chemical Accuracy in Coupled Cluster?. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4014-4020.	5.3	3
661	Delocalization of the Unpaired Electron in the Quercetin Radical: Comparison of Experimental ESR Data with DFT Calculations. <i>International Journal of Molecular Sciences</i> , 2020, 21, 2033.	4.1	11
662	Transient proton transfer of base pair hydrogen bonds induced by intense terahertz radiation. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9316-9321.	2.8	17
663	Density Functionals for Hydrogen Storage: Defining the H2Bind275 Test Set with Ab Initio Benchmarks and Assessment of 55 Functionals. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4963-4982.	5.3	14
664	Revisiting diacetyl and acetic acid flames: The role of the ketene+OH reaction. <i>Combustion and Flame</i> , 2020, 218, 28-41.	5.2	13
665	A comparison of DLPNO-CCSD(T) and CCSD(T) method for the determination of the energetics of hydrogen atom transfer reactions. <i>Computational and Theoretical Chemistry</i> , 2020, 1187, 112934.	2.5	34
666	Difficulties of Popular Density Functionals to Describe the Conformational Isomerism in Iodoacetic Acid. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5570-5579.	2.5	2
667	Color tuning of an active pharmaceutical ingredient through cocrystallization: a case study of a metronidazole–pyrogallol cocrystal. <i>CrystEngComm</i> , 2020, 22, 1404-1413.	2.6	19

#	ARTICLE	IF	CITATIONS
668	Performance of Electronic Structure Methods for the Description of H ₂ and H ₂ ⁺ Interconversions in Extended π -Systems. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2380-2397.	2.5	22
669	Mechanistic Studies of Bioorthogonal ATP Analogues for Assessment of Histidine Kinase Autophosphorylation. <i>ACS Chemical Biology</i> , 2020, 15, 1252-1260.	3.4	11
670	Unusual Racemization of Tertiary P- π -Chiral Ferrocenyl Phosphines. <i>Chemistry - A European Journal</i> , 2020, 26, 5765-5769.	3.3	5
671	Chemical promenades: Exploring potential energy surfaces with immersive virtual reality. <i>Journal of Computational Chemistry</i> , 2020, 41, 1310-1323.	3.3	21
672	Density-functional tight-binding: basic concepts and applications to molecules and clusters. <i>Advances in Physics: X</i> , 2020, 5, 1710252.	4.1	53
673	Electrocatalytic Hydrogen Evolution and Oxidation with Rhenium Tris(thiolate) Complexes: A Competition between Rhenium and Sulfur for Electrons and Protons. <i>ACS Catalysis</i> , 2020, 10, 3778-3789.	11.2	22
674	Synthesis and Conformational Analysis of Parent Perhydroazulenes Reveal an Energetically Preferred cis Ring Fusion. <i>Journal of Organic Chemistry</i> , 2020, 85, 4441-4447.	3.2	9
675	Mechanism of Ir-catalyzed hydrogenation: A theoretical view. <i>Coordination Chemistry Reviews</i> , 2020, 412, 213251.	18.8	33
676	Physical mechanism of concentration-dependent fluorescence resonance energy transfer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 231, 118143.	3.9	6
677	On the mechanism of soot nucleation. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5314-5331.	2.8	136
678	Theoretical studies on the N π -X (X = Cl, O) bond activation mechanism in catalytic C-H amination. <i>Catalysis Science and Technology</i> , 2020, 10, 1914-1924.	4.1	5
679	Toward Fully Unsupervised Anharmonic Computations Complementing Experiment for Robust and Reliable Assignment and Interpretation of IR and VCD Spectra from Mid-IR to NIR: The Case of 2,3-Butanediol and <i>trans</i> -1,2-Cyclohexanediol. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1011-1024.	2.5	26
680	Modelling Enzymatic Mechanisms with QM/MM Approaches: Current Status and Future Challenges. <i>Israel Journal of Chemistry</i> , 2020, 60, 655-666.	2.3	40
681	Bayesian Optimization for Calibrating and Selecting Hybrid-Density Functional Models. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4053-4061.	2.5	107
682	The ONIOM/PMM Model for Effective Yet Accurate Simulation of Optical and Chiroptical Spectra in Solution: Camphorquinone in Methanol as a Case Study. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3294-3306.	5.3	17
683	Double hybrid \langle scf \rangle DFT \langle /scf \rangle calculations with Slater type orbitals. <i>Journal of Computational Chemistry</i> , 2020, 41, 1660-1684.	3.3	16
684	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3041-3054.	5.3	21
685	What Determines the Glass Temperature and dc-Conductivity in Imidazolium-Polymerized Ionic Liquids with a Polythiophene Backbone?. <i>Macromolecules</i> , 2020, 53, 3535-3550.	4.8	18

#	ARTICLE	IF	CITATIONS
686	Appraising spin-state energetics in transition metal complexes using double-hybrid models: accountability of SOS0-PBESCAN0-2(a) as a promising paradigm. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9388-9404.	2.8	10
687	Computation of covalent and noncovalent structural parameters at low computational cost: Efficiency of the $\text{DH}\hat{\text{SVPD}}$ method. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26233.	2.0	7
688	A density functional theory study of the stereoselectivity of $\text{Cu}(\text{OTf})_2$ -catalyzed [3+2] cycloaddition of trifluoromethylated <i>N</i> -acylhydrazones and isoprene: A concerted asynchronous mechanism. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26236.	2.0	1
689	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of SIE and NCE . <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, .	14.6	25
690	The Trip to the Density Functional Theory Zoo Continues: Making a Case for Time-Dependent Double Hybrids for Excited-State Problems. <i>Australian Journal of Chemistry</i> , 2021, 74, 3.	0.9	39
691	Combined experimental and quantum mechanical elucidation of the synthetically accessible stereoisomers of Hydroxyestradienone (HED), the starting material for vilaprisan synthesis. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 505-516.	2.9	0
692	Strain-Driven Dyotropic Rearrangement: A Unified Ring-Expansion Approach to \pm -Methylene- β -butyrolactones. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 4221-4230.	13.8	21
693	Fitting elephants in the density functionals zoo: Statistical criteria for the evaluation of density functional theory methods as a suitable replacement for counting parameters. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26379.	2.0	7
694	Spin-Controlled Binding of Carbon Dioxide by an Iron Center: Insights from Ultrafast Mid-Infrared Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 2519-2525.	13.8	10
695	The hydrogen-bond configuration modulates the energy transfer efficiency in helical protein nanotubes. <i>Nanoscale</i> , 2021, 13, 991-999.	5.6	6
696	Theoretical study on conformational energies of transition metal complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 287-299.	2.8	52
697	SAMPL7: Host-guest binding prediction by molecular dynamics and quantum mechanics. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 63-77.	2.9	9
698	Strain-Driven Dyotropic Rearrangement: A Unified Ring-Expansion Approach to \pm -Methylene- β -butyrolactones. <i>Angewandte Chemie</i> , 2021, 133, 4267-4276.	2.0	2
699	Spin-Controlled Binding of Carbon Dioxide by an Iron Center: Insights from Ultrafast Mid-Infrared Spectroscopy. <i>Angewandte Chemie</i> , 2021, 133, 2549-2555.	2.0	2
700	Directed Gas Phase Formation of the Elusive Silylgermylidyne Radical (H_3SiGe , X_2Ae^2). <i>ChemPhysChem</i> , 2021, 22, 184-191.	2.1	3
701	Can density functional theory $\hat{\text{Cope}}^{\text{TM}}$ with highly fluxional shapeshifting molecules?. <i>Chemical Physics</i> , 2021, 540, 111013.	1.9	15
702	Conformational energies and equilibria of cyclic dinucleotides <i>in vacuo</i> and in solution: computational chemistry <i>vs.</i> NMR experiments. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7280-7294.	2.8	5
703	Benchmarking London dispersion corrected density functional theory for noncovalent ion- π interactions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11635-11648.	2.8	31

#	ARTICLE	IF	CITATIONS
704	A molecular beam and computational study on the barrierless gas phase formation of (iso)quinoline in low temperature extraterrestrial environments. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18495-18505.	2.8	5
705	Mechanistic understanding of the Cu(i)-catalyzed domino reaction constructing 1-aryl-1,2,3-triazole from electron-rich aryl bromide, alkyne, and sodium azide: a DFT study. <i>Catalysis Science and Technology</i> , 2021, 11, 3208-3216.	4.1	3
706	Study of the structural and optoelectronic properties of dye solar cells based on phosphonic acid anchoring by DFT functionals. <i>New Journal of Chemistry</i> , 2021, 45, 2723-2733.	2.8	12
707	A Simple Range-Separated Double-Hybrid Density Functional Theory for Excited States. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 927-942.	5.3	38
708	Electronic and geometric determinants of adsorption: fundamentals and applications. <i>JPhys Energy</i> , 2021, 3, 022001.	5.3	18
709	Assessing the Applicability of the Geometric Counterpoise Correction in B2PLYP/Double- ζ Calculations for Thermochemistry, Kinetics, and Noncovalent Interactions*. <i>Australian Journal of Chemistry</i> , 2021, , .	0.9	2
710	A rotational spectroscopic and <i>ab initio</i> study of <i>cis</i> - and <i>trans</i> -(α)-carveol: further insights into conformational dynamics in monoterpenes and monoterpenoids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15159-15168.	2.8	6
711	The solvation structure, transport properties and reduction behavior of carbonate-based electrolytes of lithium-ion batteries. <i>Chemical Science</i> , 2021, 12, 14740-14751.	7.4	29
712	How many shades of grey? On the proximity of density functional approximation to <i>ab initio</i> method via calculations of electric multipole moments. <i>Journal of Physics: Conference Series</i> , 2021, 1730, 012126.	0.4	0
713	Picture-change correction in relativistic density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15458-15474.	2.8	1
714	Commentary toward the 20th Anniversary of the Society of Computer Chemistry, Japan. <i>Journal of Computer Chemistry Japan</i> , 2021, 20, A26-A40.	0.1	0
715	Vibrational dynamics of hydrogen molecules under intense THz waves. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, 70, 243101.	0.5	0
716	A Computational Analysis of the Reaction of Atomic Oxygen O(3P) with Acrylonitrile. <i>Lecture Notes in Computer Science</i> , 2021, , 339-350.	1.3	0
717	A general QSPR protocol for the prediction of atomic/inter-atomic properties: a fragment based graph convolutional neural network (F-GCN). <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13242-13249.	2.8	9
718	Singlet and Triplet Contributions to the Excited-State Activities of Dihydrophenazine, Phenoxazine, and Phenothiazine Organocatalysts Used in Atom Transfer Radical Polymerization. <i>Journal of the American Chemical Society</i> , 2021, 143, 3613-3627.	13.7	39
719	QUESTDB: A database of highly accurate excitation energies for the electronic structure community. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1517.	14.6	84
720	Too big, too small, or just right? A benchmark assessment of density functional theory for predicting the spatial extent of the electron density of small chemical systems. <i>Journal of Chemical Physics</i> , 2021, 154, 074109.	3.0	15
721	Formation and Infrared Spectrum of the Open-Form 2-Bromoethyl Radical (2-C ₂ H ₄ Br•) from Ultraviolet Irradiation of a C ₂ H ₄ /Br ₂ /p-H ₂ Matrix. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2139-2145.	2.5	3

#	ARTICLE	IF	CITATIONS
722	Exploring the Limits of the XYG3-Type Doubly Hybrid Approximations for the Main-Group Chemistry: The xDH@B3LYP Model. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2638-2644.	4.6	17
723	Assessing challenging intra- and intermolecular charge-transfer excitations energies with double-hybrid density functionals. <i>Journal of Computational Chemistry</i> , 2021, 42, 970-981.	3.3	22
724	Judicious design functionalized 3D-COF to enhance CO ₂ adsorption and separation. <i>Journal of Computational Chemistry</i> , 2021, 42, 888-896.	3.3	14
725	Accurate Receptor-Ligand Binding Free Energies from Fast QM Conformational Chemical Space Sampling. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3078.	4.1	14
726	Theoretical insights into the direct radical scavenging activities of 8-hydroxyquinoline: Mechanistic, thermodynamic and kinetic studies. <i>Computational and Theoretical Chemistry</i> , 2021, 1198, 113174.	2.5	4
727	Exploring influence of fluorine substitution on the strength and nature of halogen bond between iodobenzene and hydrogen cyanide. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4213.	1.9	3
728	CHAL336 Benchmark Set: How Well Do Quantum-Chemical Methods Describe Chalcogen-Bonding Interactions?. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2783-2806.	5.3	42
729	Linear-Scaling Open-Shell MP2 Approach: Algorithm, Benchmarks, and Large-Scale Applications. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2886-2905.	5.3	16
730	Polarity Matters: Dielectric Relaxation in All-cis-Multifluorinated Cycloalkanes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3700-3709.	2.6	6
731	Effect of H ₂ O Molecules on the CO ₂ Replacement in CH ₄ Hydrate Behavior by Molecular Simulation. <i>Energy & Fuels</i> , 2021, 35, 8126-8140.	5.1	8
732	Kinetics of Azanone (HNO) Reactions with Thiols: Effect of pH. <i>Cell Biochemistry and Biophysics</i> , 2021, 79, 845-856.	1.8	4
733	Noncovalent Interactions from Models for the Møller-Plesset Adiabatic Connection. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4867-4875.	4.6	15
734	Assessment of Performance of Density Functionals for Predicting Potential Energy Curves in Hydrogen Storage Applications. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4245-4257.	2.5	2
735	Analysis of Recent BLYP- and PBE-Based Range-Separated Double-Hybrid Density Functional Approximations for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4026-4035.	2.5	31
736	Catalytic hydrolysis mechanism of aminocarboxylester substrate by human carboxylesterase 1: A theoretical study on methylphenidate hydrolysis. <i>Computational and Theoretical Chemistry</i> , 2021, 1199, 113198.	2.5	0
737	Interplay of Rotational and Pseudorotational Motions in Flexible Cyclic Molecules. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4098-4113.	2.5	4
738	Shermo: A general code for calculating molecular thermochemistry properties. <i>Computational and Theoretical Chemistry</i> , 2021, 1200, 113249.	2.5	331
739	Catalyst-Controlled Regiodivergence in Rearrangements of Indole-Based Onium Ylides. <i>Journal of the American Chemical Society</i> , 2021, 143, 9016-9025.	13.7	27

#	ARTICLE	IF	CITATIONS
740	Spin-Opposite-Scaled Range-Separated Exchange Double-Hybrid Models (SOS-RSX-DHs): Marriage Between DH and RSX/SOS-RSX Is Not Always a Happy Match. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4077-4091.	5.3	7
741	Combined Crossed Molecular Beams and Ab Initio Study of the Bimolecular Reaction of Ground State Atomic Silicon (Si; 3 P) with Germane (GeH ₄ ; X 1 A 1). <i>ChemPhysChem</i> , 2021, 22, 1497-1504.	2.1	1
742	Spin-Scaled Range-Separated Double-Hybrid Density Functional Theory for Excited States. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4211-4224.	5.3	25
743	Role of Dispersion Interactions in Endohedral TM@(ZnS) ₁₂ Structures. <i>ACS Omega</i> , 2021, 6, 16612-16622.	3.5	0
744	Stable High-Capacity Organic Aluminum-Porphyrin Batteries. <i>Advanced Energy Materials</i> , 2021, 11, 2101446.	19.5	54
745	Time-Dependent Long-Range-Corrected Double-Hybrid Density Functionals with Spin-Component and Spin-Opposite Scaling: A Comprehensive Analysis of Singlet-Singlet and Singlet-Triplet Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5165-5186.	5.3	58
746	Catalytic S _N Ar Hydroxylation and Alkoxylation of Aryl Fluorides. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20391-20399.	13.8	22
747	Density Functional Theory for Electrocatalysis. <i>Energy and Environmental Materials</i> , 2022, 5, 157-185.	12.8	95
748	Energies, structures, and harmonic frequencies of small water clusters from the direct random phase approximation. <i>Journal of Chemical Physics</i> , 2021, 155, 084303.	3.0	1
749	Directed Gas-Phase Formation of Aminosilylene (HSiNH ₂ X ⁺¹): The Simplest Silicon Analogue of an Aminocarbene, under Single-Collision Conditions. <i>Journal of the American Chemical Society</i> , 2021, 143, 14227-14234.	13.7	6
750	Initial Decomposition Mechanism of 3-Nitro-1,2,4-triazol-5-one (NTO) under Shock Loading: ReaxFF Parameterization and Molecular Dynamic Study. <i>Molecules</i> , 2021, 26, 4808.	3.8	14
751	Active Thermochemical Tables: the thermophysical and thermochemical properties of methyl, CH ₃ , and methylene, CH ₂ , corrected for nonrigid rotor and anharmonic oscillator effects. <i>Molecular Physics</i> , 0, , e1969046.	1.7	12
752	Catalytic S _N Ar Hydroxylation and Alkoxylation of Aryl Fluorides. <i>Angewandte Chemie</i> , 2021, 133, 20554-20562.	2.0	4
753	Extrapolating DFT Toward the Complete Basis Set Limit: Lessons from the PBE Family of Functionals. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5651-5660.	5.3	14
754	Tautomeric equilibrium, proton affinity and mass spectrometry fragmentation of flexible hydrogen-bonded precursors and rigid $\{N\} \rightarrow \{BF\}_2$ fluorescent dyes. <i>Scientific Reports</i> , 2021, 11, 15995.	3.3	2
755	On assessing functional errors in density functional theory using atomisation energies and electric field gradients. <i>International Journal of Quantum Chemistry</i> , 0, , e26799.	2.0	1
756	MCML: Combining physical constraints with experimental data for a multi-purpose meta-generalized gradient approximation. <i>Journal of Computational Chemistry</i> , 2021, 42, 2004-2013.	3.3	10
757	A subtle structure evolution of metal-adsorbed water bilayer and the effect of dispersion correction. <i>Computational Materials Science</i> , 2021, 196, 110533.	3.0	3

#	ARTICLE	IF	CITATIONS
758	High performance SACs for HER process using late first-row transition metals anchored on graphyne support: A DFT insight. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 37814-37823.	7.1	49
759	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6134-6151.	5.3	75
760	2-Methylfuran (MF) as a potential biofuel: A thorough review on the production pathway from biomass, combustion progress, and application in engines. <i>Renewable and Sustainable Energy Reviews</i> , 2021, 148, 111265.	16.4	96
761	Computational insights into the reactivity of chlorpyrifos and chlorpyrifos-methyl toward singlet oxygen. <i>Journal of Molecular Modeling</i> , 2021, 27, 282.	1.8	0
762	Synthesis, Crystal and Electronic Structures of a Thiophosphinoyl- and Amino-Substituted Metallated Ylide. <i>ChemistryOpen</i> , 2021, 10, 1089-1094.	1.9	6
763	Deep eutectic solvents formed by EmimCl plus lactams: Effective SO ₂ capture and conversion into sulphur via DESs-mediated Claus process. <i>Chemical Engineering Journal</i> , 2021, 422, 130033.	12.7	28
764	Assessment of density functional theory in studying on the transition states of a Diiron-mediated N N bond cleavage reaction. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113418.	2.5	1
765	Reticular chemistry approach to explore the catalytic CO ₂ -epoxide cycloaddition reaction over tetrahedral coordination Lewis acidic sites in a Rutile-type Zinc-phosphonocarboxylate framework. <i>Chemical Engineering Journal</i> , 2022, 427, 131759.	12.7	20
766	Orbital transitions: insight into energy transfer through an antenna for an organo-lanthanide complex. <i>Chemical Communications</i> , 2021, 57, 10727-10730.	4.1	0
767	SAMPL7 Host-Guest Challenge Overview: assessing the reliability of polarizable and non-polarizable methods for binding free energy calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 1-35.	2.9	45
768	The bimetallic and the anchoring group effects on both optical and charge transport properties of hexaphyrin amethyrin. <i>New Journal of Chemistry</i> , 2021, 45, 6521-6534.	2.8	4
769	High-throughput virtual screening for organic electronics: a comparative study of alternative strategies. <i>Journal of Materials Chemistry C</i> , 2021, 9, 13557-13583.	5.5	20
770	What Next for Quantum Mechanics in Structure-Based Drug Discovery?. <i>Methods in Molecular Biology</i> , 2020, 2114, 339-353.	0.9	11
771	A Computational Study of the Reaction Cyanoacetylene and Cyano Radical Leading to 2-Butynedinitrile and Hydrogen Radical. <i>Lecture Notes in Computer Science</i> , 2020, , 707-716.	1.3	3
772	A New Generation of Doubly Hybrid Density Functionals (DHDFs). <i>Springer Briefs in Molecular Science</i> , 2014, , 25-45.	0.1	2
773	First Steps Towards Quantum Refinement of Protein X-Ray Structures. , 2012, , 87-120.		7
774	Structure and stability of sodium-doped helium snowballs through DFT calculations. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	5
775	Pseudorotation in cyclooctane, using spherical conformational landscape model. <i>Computational and Theoretical Chemistry</i> , 2020, 1184, 112845.	2.5	3

#	ARTICLE	IF	CITATIONS
776	Crystal Growth Kinetics of a Metastable Polymorph of Tolbutamide in Organic Solvents. <i>Crystal Growth and Design</i> , 2020, 20, 1985-1996.	3.0	14
778	Unraveling Conformer-Specific Sources of Hydroxyl Radical Production from an Isoprene-Derived Criegee Intermediate by Deuteration. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4929-4938.	2.5	10
779	Comparing the performances of various density functionals for modelling the mechanisms and kinetics of bimolecular free radical reactions in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23425-23440.	2.8	7
780	A way of resolving the order-of-limit problem of Tao's Mo semilocal functional. <i>Journal of Chemical Physics</i> , 2020, 153, 184112.	3.0	15
781	Large coupling-strength expansion of the Møller-Plesset adiabatic connection: From paradigmatic cases to variational expressions for the leading terms. <i>Journal of Chemical Physics</i> , 2020, 153, 214112.	3.0	16
782	Different bonding type along each crystallographic axis: Computational study of poly(p-phenylene) Tj ETQq1 1 0.784314 rgBT /Overl	2.4	7
783	Study of stacking interactions between two neutral tetrathiafulvalene molecules in Cambridge Structural Database crystal structures and by quantum chemical calculations. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 1-7.	1.1	9
784	Hydrogen atom transfer rates from Tp-containing metal-hydrides to trityl radicals. <i>Canadian Journal of Chemistry</i> , 2021, 99, 216-220.	1.1	5
786	Thiosemicarbazones Synthesized from Acetophenones: Tautomerism, Spectrometric Data, Reactivity and Theoretical Calculations. <i>International Journal of Analytical Mass Spectrometry and Chromatography</i> , 2019, 07, 19-34.	0.7	5
787	Why the Standard B3LYP/6-31G* Model Chemistry Should Not Be Used in DFT Calculations of Molecular Thermochemistry: Understanding and Correcting the Problem. <i>Journal of Organic Chemistry</i> , 2012, 77, 10824-10834.	3.2	14
788	Theoretical Study on Terahertz Oscillation of Protons in Zundel Cations. , 2021, , .		0
789	Theory and Experiment Demonstrate that Sb(V)-Promoted Methane C-H Activation and Functionalization Outcompete Superacid Protonolysis in Sulfuric Acid. <i>Journal of the American Chemical Society</i> , 2021, 143, 18242-18250.	13.7	8
790	Benchmarking the Performance of DHDFs for the Main Group Chemistry. <i>Springer Briefs in Molecular Science</i> , 2014, , 47-77.	0.1	0
791	An Overview of Modern Density Functional Theory. <i>Springer Briefs in Molecular Science</i> , 2014, , 1-24.	0.1	0
792	GC/MS Analyses of Thiosemicarbazones Synthesized from Acetophenones: Thermal Decay and Mass Spectra Features. <i>International Journal of Analytical Mass Spectrometry and Chromatography</i> , 2015, 03, 1-13.	0.7	1
793	The Ethanol Tree: Gas-Phase Formation Routes for Glycolaldehyde, Its Isomer Acetic Acid and Formic Acid. <i>Lecture Notes in Computer Science</i> , 2018, , 730-745.	1.3	2
795	MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling. , 2020, , 523-543.		0
796	Crystal and geometry-optimized structure of an anthracene-based Diels-Alder adduct. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 639-646.	0.5	0

#	ARTICLE	IF	CITATIONS
797	Gas-phase Synthesis of Silaformaldehyde (H_2SiO) and Hydroxysilylene (HSiOH) in Outflows of Oxygen-rich Asymptotic Giant Branch Stars. <i>Astrophysical Journal Letters</i> , 2021, 921, L7.	8.3	0
798	In-situ polymerized solid-state electrolytes with stable cycling for Li/LiCoO ₂ batteries. <i>Nano Energy</i> , 2022, 91, 106679.	16.0	62
799	Understanding the effect of antisolvent on processing window and efficiency for large-area flexible perovskite solar cells. <i>Materials Today Physics</i> , 2021, 21, 100565.	6.0	9
800	Comment on “Exploring nature and predicting strength of hydrogen bonds: A correlation analysis between atoms-in-molecules descriptors, binding energies, and energy components of symmetry-adapted perturbation theory”. <i>Journal of Computational Chemistry</i> , 2021, 42, 516-521.	3.3	9
801	A Theoretical Investigation of the Reaction Between Glycolaldehyde and H^+ and Implications for the Organic Chemistry of Star Forming Regions. <i>Lecture Notes in Computer Science</i> , 2020, , 730-743.	1.3	0
802	Exploring Guest-Host Interactions in Gas Hydrates: Insights from Quantum Mechanics. <i>Energy & Fuels</i> , 2021, 35, 18604-18614.	5.1	5
804	A theoretical study for the role of complex in hydrogen abstraction of OH. <i>Chemical Physics Letters</i> , 2020, 759, 138035.	2.6	1
805	Effect of confinement on the dynamics of 1-propanol and other monohydroxy alcohols. <i>Journal of Chemical Physics</i> , 2021, 155, 184504.	3.0	8
806	Interfacial layer rich in organic fluoride enabling stable cycling of high-voltage PEO-based solid-state lithium batteries. <i>Electrochimica Acta</i> , 2022, 404, 139617.	5.2	5
807	New preparation protocols for coumarin-thiosemicarbazone hybrids: Solid state characterization, and in silico/NMR studies of the Z/E isomerization equilibria in solution. <i>Journal of Molecular Structure</i> , 2022, 1251, 131980.	3.6	5
808	Evidences for sulfur centered hydrogen bond with sulfur atoms as a donor in aromatic thiols and aliphatic thiols in aqueous solution. <i>Journal of Molecular Liquids</i> , 2022, 348, 118078.	4.9	13
809	Glycolonitrile (HOCH_2CN) Chemistry in Star-forming Regions. <i>Astrophysical Journal, Supplement Series</i> , 2021, 257, 26.	7.7	4
810	Electro-catazone treatment of ozone-resistant drug ibuprofen: Interfacial reaction kinetics, influencing mechanisms, and degradation sites. <i>Journal of Hazardous Materials Advances</i> , 2021, 4, 100023.	3.0	7
811	Structural and Energetic Properties of Amino Acids and Peptides Benchmarked by Accurate Theoretical and Experimental Data. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9826-9837.	2.5	6
812	Zinc(II) Iodide-Directed I^2 -Mannosylation: Reaction Selectivity, Mode, and Application. <i>Journal of Organic Chemistry</i> , 2021, 86, 16901-16915.	3.2	8
813	Benchmark calculations and error cancelations for bond dissociation enthalpies of XNO_2 . <i>Defence Technology</i> , 2023, 22, 144-155.	4.2	6
814	Kinetic Study on the Reactivity of Azanone (HNO) toward Cyclic C-Nucleophiles. <i>International Journal of Molecular Sciences</i> , 2021, 22, 12982.	4.1	6
815	Inception of Carbonaceous Nanostructures via Hydrogen-Abstraction Phenylacetylene-Addition Mechanism. <i>Journal of the American Chemical Society</i> , 2021, 143, 20710-20716.	13.7	12

#	ARTICLE	IF	CITATIONS
816	A Theoretical Investigation into the Comparative Adsorption Between Dissolved Oxygen and Oxygenate Species on Zeolite 3.7 Å... During Aviation Fuel Treatment for Thermal Stability Improvement. SSRN Electronic Journal, 0, , .	0.4	0
817	Ternary complexes of chiral disulfonimides in transfer-hydrogenation of imines: the relevance of late intermediates in ion pair catalysis. Chemical Science, 2021, 12, 15263-15272.	7.4	10
818	New insights into the capture performance and mechanism of hazardous metals Cr ³⁺ and Cd ²⁺ onto an effective layered double hydroxide based material. Journal of Hazardous Materials, 2022, 426, 128062.	12.4	155
819	High-valent iron-oxo species mediated cyclic oxidation through single-atom Fe-N ₆ sites with high peroxymonosulfate utilization rate. Applied Catalysis B: Environmental, 2022, 305, 121049.	20.2	48
820	Reliability of computed molecular structures. Journal of Computational Chemistry, 2022, 43, 465-476.	3.3	3
821	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. Angewandte Chemie - International Edition, 2022, 61, .	13.8	19
822	Elucidating the selectivity of dyotropic rearrangements of β^2 -lactones: a computational survey. Organic Chemistry Frontiers, 2022, 9, 329-341.	4.5	6
823	Carbon π -Iron Electron Transport Channels in Porphyrin π -Graphene Complex for ppb μ -level Room Temperature NO Gas Sensing. Small, 2022, 18, e2103259.	10.0	12
824	Accurate Spectral Properties within Double-Hybrid Density Functional Theory: A Spin-Scaled Range-Separated Second-Order Algebraic-Diagrammatic Construction-Based Approach. Journal of Chemical Theory and Computation, 2022, 18, 865-882.	5.3	14
825	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. Angewandte Chemie, 0, , .	2.0	6
826	Chalcogen π - π -Chalcogen Bonding in Molybdenum Disulfide, Molybdenum Diselenide and Molybdenum Diteelluride Dimers as Prototypes for a Basic Understanding of the Local Interfacial Chemical Bonding Environment in 2D Layered Transition Metal Dichalcogenides. Inorganics, 2022, 10, 11.	2.7	8
827	Reaction kinetics of phenyl π - π phenylacetylene at combustion-relevant intermediate temperatures. Combustion and Flame, 2022, 243, 112014.	5.2	4
828	Do any types of double-hybrid models render the correct order of excited state energies in inverted singlet π -triplet emitters?. Journal of Chemical Physics, 2022, 156, 064302.	3.0	6
829	Accurate redox potentials for solvents in $\langle \text{scp} \rangle \text{Li}^{\text{metal}} \langle \text{scp} \rangle$ batteries and assessment of density functionals. International Journal of Quantum Chemistry, 2022, 122, .	2.0	6
830	The unexpected crystal structure of thallium(I) tricyanomethanide Tl[C(CN) ₃]. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2022, .	0.7	0
831	A theoretical investigation into the comparative adsorption between dissolved oxygen and oxygenate species on zeolite 3.7Å...Åduring aviation fuel treatment for thermal stability improvement. Fuel, 2022, 317, 123451.	6.4	2
832	Natural Quinone Molecules as Effective Cath Ode Materials for Lithium-Ion Batteries: A First-Principles Study. SSRN Electronic Journal, 0, , .	0.4	0
833	Theoretical study for evaluating and discovering organic hydride compounds as novel trifluoromethylation reagents. Organic and Biomolecular Chemistry, 2022, 20, 2831-2842.	2.8	5

#	ARTICLE	IF	CITATIONS
834	C(sp ³)â€”H Amination Catalyzed by Ir(Me)-Porphyrin: A Computational Study. <i>Organometallics</i> , 2022, 41, 569-580.	2.3	4
835	Diverse Secondary Metabolites from the Coral-Derived Fungus <i>Aspergillus hiratsukae</i> SCSIO 5Bn1003. <i>Marine Drugs</i> , 2022, 20, 150.	4.6	4
836	Investigation on the Lithium Extraction Process with the TBPâ€”FeCl ₃ Solvent System Using Experimental and DFT Methods. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 4672-4682.	3.7	18
837	Additive Engineering in Antisolvent for Widening the Processing Window and Promoting Perovskite Seed Formation in Perovskite Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 17348-17357.	8.0	9
838	Protocol for Directing Nudged Elastic Band Calculations to the Minimum Energy Pathway: Nurturing Errant Calculations Back to Convergence. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2993-3005.	5.3	8
839	Natural quinone molecules as effective cathode materials for nonaqueous lithium-ion batteries. <i>Journal of Power Sources</i> , 2022, 531, 231291.	7.8	15
840	Isotope Effects on the Vaporization of Organic Compounds from an Aqueous Solutionâ€”Insight from Experiment and Computations. <i>Journal of Physical Chemistry B</i> , 2021, 125, 13868-13885.	2.6	5
841	Artificial intelligence-enhanced quantum chemical method with broad applicability. <i>Nature Communications</i> , 2021, 12, 7022.	12.8	52
842	Small-Basis Set Density-Functional Theory Methods Corrected with Atom-Centered Potentials. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2913-2930.	5.3	4
843	Mechanism of E-bridge formation by various PAH molecules: A theoretical study. <i>Chemical Physics Letters</i> , 2022, 799, 139637.	2.6	5
844	Borole/Borapyramidane Relationship. <i>Journal of the American Chemical Society</i> , 2022, 144, 7815-7821.	13.7	10
845	A missing link in the nitrogen-rich organic chain on Titan. <i>Astronomy and Astrophysics</i> , 2022, 663, A165.	5.1	1
846	Do Double-Hybrid Functionals Benefit from Regularization in the PT2 Term? Observations from an Extensive Benchmark. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3499-3506.	4.6	14
847	Rhodium-based bidentate phosphorus ligand catalyst for direct synthesis of ethylene glycol. <i>Molecular Catalysis</i> , 2022, 524, 112288.	2.0	0
848	The role of intermolecular interactions of aromatic sandwich dimer ligands for the half-titanocene catalysts: Theoretical study. <i>Chemical Physics</i> , 2022, 559, 111556.	1.9	0
849	Computational study of ground-state properties of $\langle i \rangle^{1/4} \langle i \rangle^{-2}$ â€”bridged group 14 porphyrinic sandwich complexes. <i>Journal of Computational Chemistry</i> , 2022, , .	3.3	1
850	Computational studies on the possible formation of glycine <i>via</i> open shell gas-phase chemistry in the interstellar medium. <i>Organic and Biomolecular Chemistry</i> , 2022, , .	2.8	2
851	Noncovalently bound excited-state dimers: a perspective on current time-dependent density functional theory approaches applied to aromatic excimer models. <i>RSC Advances</i> , 2022, 12, 13014-13034.	3.6	18

#	ARTICLE	IF	CITATIONS
852	Molecular docking assisted exploration on solubilization of poorly soluble drug remdesivir in sulfobutyl ether-tycyclodextrin. AAPS Open, 2022, 8, 9.	1.3	3
853	A New Enthalpy of Formation Test Set Designed for Organic Fluorine Containing Compounds. Advanced Theory and Simulations, 0, , 2200093.	2.8	1
854	Density-functional <i>theory</i> vs density-functional fits. Journal of Chemical Physics, 2022, 156, .	3.0	19
855	Conformational Energy Benchmark for Longer <i>n</i>-Alkane Chains. Journal of Physical Chemistry A, 2022, 126, 3521-3535.	2.5	16
856	A quantum-chemistry and molecular-dynamics study of non-covalent interactions between tri-n-butyl phosphate and 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. Journal of Molecular Liquids, 2022, 360, 119430.	4.9	8
857	1,2,3-Oxaphosphetanes and Their P-Chalcogenides—A Combined Experimental and Theoretical Study. Molecules, 2022, 27, 3345.	3.8	1
858	Dissociation of Bipyridine and Coordination with Nitrosyl: Cyclometalated Ruthenium Nitrosyl Complex. Inorganic Chemistry, 2022, 61, 8997-9011.	4.0	5
859	Analytic Gradients for the Long-Range-Corrected XYG3 Type of Doubly Hybrid Density Functionals: Theory, Implementation, and Assessment. Journal of Physical Chemistry A, 2022, 126, 3937-3946.	2.5	1
861	Inverse molecular design of alkoxides and phenoxides for aqueous direct air capture of CO ₂ . Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	8
862	Electron transfer accelerated polymer-TiO ₂ coatings for enhanced photocatalytic activity in photocathodic protection. Applied Surface Science, 2022, 599, 153984.	6.1	6
863	Maximally exploiting active sites on Yolk@shell nanoreactor: Nearly 100% PMS activation efficiency and outstanding performance over full pH range in Fenton-like reaction. Applied Catalysis B: Environmental, 2022, 316, 121594.	20.2	73
864	Antibacterial silver and gold complexes of imidazole and 1,2,4-triazole derived N-heterocyclic carbenes. Dalton Transactions, 2022, 51, 12056-12070.	3.3	6
865	Delocalization error: The greatest outstanding challenge in density-functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	14.6	43
866	The Photoionization Dynamics, Electronic Spectroscopy, and Excited State Photochemistry of AlCO and AlOC. Astrophysical Journal, 2022, 933, 192.	4.5	3
867	A Look at Real-World Transition-Metal Thermochemistry and Kinetics with Local Hybrid Functionals. Israel Journal of Chemistry, 2023, 63, .	2.3	8
868	Fullerenes Pose a Strain on Hybrid Density Functional Theory. Journal of Physical Chemistry A, 2022, 126, 4709-4720.	2.5	5
869	High-Level Quantum Chemistry Reference Heats of Formation for a Large Set of C, H, N, and O Species in the NIST Chemistry Webbook and the Identification and Validation of Reliable Protocols for Their Rapid Computation. Journal of Physical Chemistry A, 2022, 126, 4981-4990.	2.5	13
870	The Complexation between Siloxane Species and Methylsiloxane: Electronic Structure, Thermodynamic, and Interaction Characteristics. ChemistrySelect, 2022, 7, .	1.5	0

#	ARTICLE	IF	CITATIONS
871	An assessment of orbital energy corrections for the direct random phase approximation and explicit ϵ -functionals. <i>Molecular Physics</i> , 0, , .	1.7	5
872	TMGe8-17 π (TM=Ti, Zr, Hf, V, Nb, Ta) clusters: group determined properties. <i>European Physical Journal Plus</i> , 2022, 137, .	2.6	12
873	Structural characteristics and chloride intrusion mechanism of passive film. <i>Corrosion Science</i> , 2022, 207, 110563.	6.6	17
874	Electrochemical oxidation of Naproxen in aqueous matrices: Elucidating the intermediates TM eco-toxicity, by assessing its degradation pathways via experimental and density functional theory (DFT) approaches. <i>Chemical Engineering Journal</i> , 2023, 451, 138483.	12.7	11
875	Comparison of the hydrogen extraction reactions of isopentane molecules and ions. <i>Physical Chemistry Chemical Physics</i> , 0, , .	2.8	0
876	A three dimensional graphdiyne-like porous triptycene network for gas adsorption and separation. <i>RSC Advances</i> , 2022, 12, 28299-28305.	3.6	4
877	Discovery of Cyclic Diarylheptanoids as Inhibitors against Influenza A Virus from the Roots of <i>Casuarina equisetifolia</i> . <i>Journal of Natural Products</i> , 2022, 85, 2142-2148.	3.0	1
878	Modified Magnesium Alkyls for Ziegler-Natta Catalysts. <i>Catalysts</i> , 2022, 12, 973.	3.5	2
879	A Systemic Insight into Exohedral Actinides and Endohedral Borospherenes: An&Bm and An@Bn (An=U, Np, Pu; m = 28, 32, 34, 36, 38, 40; n = 36, 38, 40). <i>Molecules</i> , 2022, 27, 6047.	3.8	3
880	The ionic salts with super oxidizing ions O ₂ ⁺ and N ₅ ⁺ : Potential candidates for high-energy oxidants. <i>Frontiers in Chemistry</i> , 0, 10, .	3.6	0
881	Roles of the Flexible Primary Coordination Sphere of the Mn ₄ CaO _x Cluster: What Are the Immediate Decay Products of the S_3 State?. <i>Journal of Physical Chemistry B</i> , 2022, 126, 7212-7228.	2.6	5
882	Explicitly Correlated Double-Hybrid DFT: A Comprehensive Analysis of the Basis Set Convergence on the GMTKN55 Database. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 5978-5991.	5.3	15
883	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	36
884	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	168
885	Regulating the Acidity of SO ₃ H-Functionalized Ionic Liquids: Hydrogen Bonding or Electrostatic Potential?. <i>ChemPlusChem</i> , 0, , .	2.8	0
886	Revisiting fundamental properties of TiO ₂ nanoclusters as condensation seeds in astrophysical environments. <i>Astronomy and Astrophysics</i> , 2022, 668, A35.	5.1	5
887	Directed gas phase preparation of ethynylallene (H ₂ CCCHCCH; X ¹) ϵ via ϵ the crossed molecular beam reaction of the methylidyne radical (CH; X ²) with vinylacetylene (H ₂ CCHCCH; X ¹). <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26499-26510.	2.8	3
888	An overview of the SAMPL8 host-guest binding challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 707-734.	2.9	17

#	ARTICLE	IF	CITATIONS
889	Non-empirical double-hybrid density functionals as reliable tools for electronic structure calculations. <i>Electronic Structure</i> , 2022, 4, 043001.	2.8	4
890	Rate constants for H-atom abstraction reactions from mono-aromatic hydrocarbons by H, CH ₃ , OH and 3O ₂ : A systematic theoretical investigation. <i>Combustion and Flame</i> , 2023, 257, 112421.	5.2	5
891	Reliable gas-phase tautomer equilibria of drug-like molecule scaffolds and the issue of continuum solvation. <i>Journal of Computer-Aided Molecular Design</i> , 0, , .	2.9	4
892	Reactivities of silane coupling agents in the silica/rubber composites: Theoretical insights into the relationships between energy barriers and electronic characteristics. <i>Journal of Computational Chemistry</i> , 2023, 44, 581-593.	3.3	1
893	The Accuracy of Semi-Empirical Quantum Chemistry Methods on Soot Formation Simulation. <i>International Journal of Molecular Sciences</i> , 2022, 23, 13371.	4.1	1
894	Accuracy of quantum chemistry structures of chiral tag complexes and the assignment of absolute configuration. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 27705-27721.	2.8	10
895	Assessment of advanced xDH@B3LYP methods in describing various potential energy curves driven by $\langle i \rangle \ddot{I} \langle i \rangle$ - $\langle i \rangle \ddot{I} \langle i \rangle$, CH/ $\langle i \rangle \ddot{I} \langle i \rangle$, and SH/ $\langle i \rangle \ddot{I} \langle i \rangle$ non-bonded interactions. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 720-726.	1.3	2
896	Carbonyl heterocycle modified mesoporous carbon nitride in photocatalytic peroxydisulfate activation for enhanced ciprofloxacin removal: Performance and mechanism. <i>Journal of Hazardous Materials</i> , 2023, 444, 130412.	12.4	9
897	Reliability of Computing van der Waals Bond Lengths of Some Rare Gas Diatomics. <i>International Journal of Molecular Sciences</i> , 2022, 23, 13944.	4.1	0
898	Libra: A modular software library for quantum nonadiabatic dynamics. <i>Software Impacts</i> , 2022, 14, 100445.	1.4	6
899	Quantum chemistry insight into the interactions of 1,3-diisopropoxycalix[4]arene-crown-6 with alkali metal cations: Structure, selectivity, and solvation. <i>Journal of Molecular Liquids</i> , 2023, 370, 121054.	4.9	4
900	Connections between the accuracy of rotational constants and equilibrium molecular structures. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1421-1429.	2.8	33
901	A comprehensive benchmark investigation of quantum chemical methods for carbocations. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1903-1922.	2.8	3
902	Application of dual-solvent extraction for separating a low-temperature coal tar: A detailed experimental and quantum chemical study. <i>Fuel</i> , 2023, 334, 126654.	6.4	3
903	Insight into boron-doped biochar as efficient metal-free catalyst for peroxydisulfate activation: Important role of -O-B-O- moieties. <i>Journal of Hazardous Materials</i> , 2023, 445, 130479.	12.4	36
904	Fragmentation modeling of gas-phase ionic liquid clusters in high-voltage electric field. <i>Fuel</i> , 2023, 335, 126919.	6.4	2
905	Reliable prediction of association (free) energies of supramolecular complexes with heavy main group elements â€” the HS13L benchmark set. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 28831-28843.	2.8	4
906	Comment on â€œMultiple locations of boron atoms in the exohedral and endohedral $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi mathvariant="normal"} \rangle C \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 60 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle$ fullereneâ€. <i>Physical Review A</i> , 2022, 106, .	2.5	3

#	ARTICLE	IF	CITATIONS
907	Spin-State Splittings in 3d Transition-Metal Complexes Revisited: Benchmarking Approximate Methods for Adiabatic Spin-State Energy Differences in Fe(II) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 7442-7456.	5.3	11
908	Novel Carbonyl Cathode for Green and Sustainable Aluminum Organic Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 53702-53710.	8.0	13
909	Effect of Hydrogen Bond Interaction on the Decomposition Temperature, Aromaticity, and Bond Order of Nonmetallic Pentazolate Salts. <i>Crystal Growth and Design</i> , 2022, 22, 7062-7073.	3.0	6
910	Bridging Electrochemistry and Photoelectron Spectroscopy in the Context of Birch Reduction: Detachment Energies and Redox Potentials of Electron, Dielectron, and Benzene Radical Anion in Liquid Ammonia. <i>Journal of the American Chemical Society</i> , 2022, 144, 22093-22100.	13.7	1
911	Ambimodal Bispericyclic [6 + 4]/[4 + 6] Transition State Competes with Diradical Pathways in the Cycloheptatriene Dimerization: Dynamics and Experimental Characterization of Thermal Dimers. <i>Journal of the American Chemical Society</i> , 2022, 144, 22251-22261.	13.7	8
912	Multiscale Modeling of Phosphate-Â-Â-Â-Contacts in RNA U-Turns Exposes Differences between Quantum-Chemical and AMBER Force Field Descriptions. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 6182-6200.	5.4	1
914	Computational Study on the Role of Zn(II) Z-Type Ligands in Facilitating Diaryl Reductive Elimination from Pt(II). <i>Organometallics</i> , 2023, 42, 16-26.	2.3	3
915	Performance of Localized-Orbital Coupled-Cluster Approaches for the Conformational Energies of Longer n -Alkane Chains. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9375-9391.	2.5	5
916	Thermochemical evaluation of adaptive and fixed density functional theory quadrature schemes. <i>Journal of Chemical Physics</i> , 2022, 157, 234106.	3.0	0
917	Supervised learning of a chemistry functional with damped dispersion. <i>Nature Computational Science</i> , 2023, 3, 48-58.	8.0	12
918	Building on the strengths of a double-hybrid density functional for excitation energies and inverted singlet-triplet energy gaps. <i>Journal of Chemical Physics</i> , 2023, 158, .	3.0	3
919	Weak and strong \ddot{I} interactions between two monomersâ€ assessed with local vibrational mode theory. <i>Canadian Journal of Chemistry</i> , 2023, 101, 615-632.	1.1	3
920	Nanoscale Surface-Enhanced Raman Spectroscopy Investigation of a Polyphenol-Based Plasmonic Nanovector. <i>Nanomaterials</i> , 2023, 13, 377.	4.1	1
921	An Imbalance in the Force: The Need for Standardized Benchmarks for Molecular Simulation. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 412-431.	5.4	4
922	Application of facilitated transfer mechanisms of SEBS/[P(14)666][TMPP] composite membrane on CH ₄ /N ₂ separation. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109243.	6.7	1
923	Theoretical Understanding of Reactions of Rhenium and Ruthenium Tris(thiolate) Complexes with Unsaturated Hydrocarbons: Noninnocent Nature of the Ligand, Mechanism, and Origin of Differential Reactivity. <i>Inorganic Chemistry</i> , 2023, 62, 2548-2560.	4.0	2
924	Exotic Reaction Dynamics in the Gas-Phase Preparation of Anthracene (C ₁₄ H ₁₀) via Spiroaromatic Radical Transients in the Indenylâ€Cyclopentadienyl Radicalâ€Radical Reaction. <i>Journal of the American Chemical Society</i> , 2023, 145, 3084-3091.	13.7	3
925	Enhancing effect of choline chloride-based deep eutectic solvents with polyols on the aqueous solubility of curcuminâ€insight from experiment and theoretical calculation. <i>Chinese Journal of Chemical Engineering</i> , 2023, 59, 160-168.	3.5	1

#	ARTICLE	IF	CITATIONS
927	Inversion Theory Leveling as a New Methodological Approach to Antioxidant Thermodynamics: A Case Study on Phenol. <i>Antioxidants</i> , 2023, 12, 282.	5.1	0
928	Double-Hybrid Density Functional Theory for Core Excitations: Theory and Benchmark Calculations. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1310-1321.	5.3	3
929	Dissecting amide-I vibrations in histidine dipeptide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 292, 122424.	3.9	0
930	A highly-stable bifunctional NiCo2S4 nanoarray@carbon paper electrode for aqueous polysulfide/iodide redox flow battery. <i>Journal of Power Sources</i> , 2023, 561, 232607.	7.8	5
931	Modeling the Photo-Absorption Properties of Noble Metal Nanoclusters: A Challenge for Density-Functional Theory. <i>Journal of Physical Chemistry C</i> , 2023, 127, 7718-7729.	3.1	2
932	Recovery of chlorogenic acid from the DES-based extract of <i>Eucommia ulmoides</i> leaves by molecularly imprinted solid-phase extraction. <i>Industrial Crops and Products</i> , 2023, 195, 116406.	5.2	3
933	A comprehensive method of ionic liquid screening and experimental verification for simultaneous separation of multiple sulfides from oil. <i>Separation and Purification Technology</i> , 2023, 315, 123714.	7.9	2
934	Electronic structure and detonation property prediction of pentazolate derivatives: Aminopentazole, diaminopentazole cations, azopentazole, and 1,2-diazopentazole. <i>Journal of Molecular Structure</i> , 2023, 1285, 135420.	3.6	5
935	Theoretical exploration of polynitrogen compounds N_6 , N_8 , N_{10} , and N_6 ions based on N_3^+ and i -cyclo- N_5^+ . <i>Journal of Energetic Materials</i> , 0, , 1-19.	2.0	3
936	Computational insights into the rational design of organic electrode materials for metal ion batteries. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2023, 13, .	14.6	5
937	Insensitive High-Energy Density Materials Based on Azazole-Rich Rings: 1,2,4-Triazole N-Oxide Derivatives Containing Isomerized Nitro and Amino Groups. <i>International Journal of Molecular Sciences</i> , 2023, 24, 3918.	4.1	3
938	Rational Design to Activate Tetrafluoromethane by Two-Coordinate Borinium. <i>Inorganic Chemistry</i> , 2023, 62, 3518-3524.	4.0	0
939	NHC-stabilised Parent Tripentyltrialenes. <i>Chemistry - A European Journal</i> , 2023, 29, .	3.3	1
940	Computational Modeling of 4d and 5d Transition Metal Catalysts. , 2024, , 601-621.		0
941	Chemical models of adenine precursors cyanamide and carbodiimide in the interstellar medium. <i>Monthly Notices of the Royal Astronomical Society</i> , 2023, 521, 1578-1589.	4.4	3
942	The Electronic Nature of Cationic Group 10 Ylidyne Complexes. <i>Inorganics</i> , 2023, 11, 129.	2.7	5
943	A density functional theory insight into the extraction mechanism of lithium recovery from alkaline brine by β -diketones. <i>AIChE Journal</i> , 2023, 69, .	3.6	2
944	A double-hybrid density functional based on good local physics with outstanding performance on the GMTKN55 database. <i>Journal of Chemical Physics</i> , 2023, 158, .	3.0	3

#	ARTICLE	IF	CITATIONS
945	Comparison of the Performance of Density Functional Methods for the Description of Spin States and Binding Energies of Porphyrins. <i>Molecules</i> , 2023, 28, 3487.	3.8	3
946	Performance of Functionals and Basis Sets in Calculating Redox Potentials of Nitrile Alkenes and Aromatic Molecules using Density Functional Theory. <i>ChemistrySelect</i> , 2023, 8, .	1.5	2
947	Spectroscopic Analysis: Calculations of Chiroptical Spectra. , 2022, , .		0
948	Predicting Magnetic Coupling and Spin-Polarization Energy in Triangulene Analogues. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 3486-3497.	5.3	3
949	Metal- π -Stabilized Thiyl Radicals Design Inspired by Elemental Periodic Extension Notion for Ligand-Based Alkene Addition. <i>Chemistry - A European Journal</i> , 0, , .	3.3	0
950	Reactivity of bis(2-chloroprop-2-enyl)sulfide in the system hydrazine hydrate/alkali: A quantum chemical insight. <i>Journal of Physical Organic Chemistry</i> , 0, , .	1.9	0
951	Complexation mechanism of crown ethers with rubidium and cesium ions using density functional theory. <i>Computational and Theoretical Chemistry</i> , 2023, 1225, 114139.	2.5	1
952	Exploring hydration mechanism of salt ions on the methane hydrate formation: Insights from experiments, QM calculations and MD simulations. <i>Chemical Engineering Science</i> , 2023, 276, 118829.	3.8	0
953	Chemistry of NH_2OH and its related species in the ISM. <i>Monthly Notices of the Royal Astronomical Society</i> , 2023, 523, 1-22.	4.4	0
954	Magneto-structural correlations of oximate-bridged dinuclear copper(II) complex: A theoretical perspective. <i>International Journal of Quantum Chemistry</i> , 0, , .	2.0	0
955	Assessing the Accuracy of Density Functional Approximations for Predicting Hydrolysis Reaction Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 3159-3171.	5.3	1
957	Oxidation of 1,3-diphenylguanidine (DPG) by goethite activated persulfate: Mechanisms, products identification and reaction sites prediction. <i>Environmental Research</i> , 2023, 232, 116308.	7.5	3
958	Experimental and Computational Determination of a $\text{Mn}^{\text{IV}}\text{Cl}$ Homolytic Bond Dissociation Free Energy: $\text{Mn}(\text{III})\text{Cl}$ -Mediated C-H Cleavage and Chlorination. <i>Journal of the American Chemical Society</i> , 2023, 145, 13384-13391.	13.7	2
959	Chemical kinetic study of the low temperature oxidation of Alkanes with a new scheme. <i>Fuel</i> , 2023, 351, 128869.	6.4	1
960	In-situ spectroscopic probe of the intrinsic structure feature of single-atom center in electrochemical CO/CO_2 reduction to methanol. <i>Nature Communications</i> , 2023, 14, .	12.8	21
961	Benchmarking Modern Density Functionals for Broad Applications in Chemistry. , 2024, , 78-93.		0
962	Reactivity and Mechanisms of Methane, Ethane, and Benzene C-H Amination with an Iodine(III) Bistriflimide Complex. <i>Organometallics</i> , 2023, 42, 1505-1512.	2.3	3
963	Hydrogen-Donor-Controlled Polybrominated Dibenzofuran (PBDF) Formation from Polybrominated Diphenyl Ether (PBDE) Photolysis in Solutions: Competition Mechanisms of Radical-Based Cyclization and Hydrogen Abstraction Reactions. <i>Environmental Science & Technology</i> , 2023, 57, 7777-7788.	10.0	1

#	ARTICLE	IF	CITATIONS
964	Mechanistic Study and Conceptual Chemical Reactivity Analysis of Hydroboration of Carbon Dioxide Catalyzed by a Manganese(I)â€Pincer Complex. <i>Inorganic Chemistry</i> , 2023, 62, 7366-7375.	4.0	1
965	A DFT investigation of the lithium extraction process under different diluent environments. <i>Chemical Engineering Science</i> , 2023, 277, 118857.	3.8	1
966	Multi-heteroatom-doping promotes molecular oxygen activation on polymeric carbon nitride for simultaneous generation of H ₂ O ₂ and degradation of oxcarbazepine. <i>Nanoscale</i> , 2023, 15, 11482-11490.	5.6	0
967	Highly accurate CCSD(T) homolytic Alâ€H bond dissociation enthalpies â€ chemical insights and performance of density functional theory. <i>Australian Journal of Chemistry</i> , 2023, , .	0.9	1
968	Nanoclusters and nanoalloys of group 13 elements (B, Al, and Ga): benchmarking of methods and analysis of their structures and energies. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 19986-20000.	2.8	2
969	A comprehensive kinetic study of the combustion mechanism of methyl isocyanate. <i>Combustion and Flame</i> , 2023, 255, 112913.	5.2	0
970	Lanthanoid coordination prompts unusually distorted pseudo-octahedral Ni ^{II} coordination in heterodinuclear Niâ€Ln complexes: synthesis, structure and understanding of magnetic behaviour through experiment and computation. <i>Dalton Transactions</i> , 2023, 52, 10402-10414.	3.3	2
971	Do Planar Tetracoordinate Fluorine Atoms Exist? Revisiting a Theoretical Prediction. <i>Journal of Physical Chemistry A</i> , 2023, 127, 5815-5822.	2.5	1
973	Right Answer for the Right Reason? Benchmarking Protocols and Pitfalls on a Ru-Metathesis Example. <i>Journal of Chemical Theory and Computation</i> , 0, , .	5.3	0
974	Infrared Spectra of (<i>Z</i>)- and (<i>E</i>)-â€CH ₂ C(CH ₃)CHI Radicals Produced upon Photodissociation of (<i>Z</i>)- and (<i>E</i>)- (CH ₂)(CH ₃)Câ€CHI in Solid <i>para</i>-Hydrogen. <i>Journal of Physical Chemistry A</i> , 2023, 127, 5986-5998.	2.5	0
975	Assessment of DFT functionals for a minimal nitrogenase [Fe(SH) ₄ H] ⁺ model employing state-of-the-art <i>ab initio</i> methods. <i>Journal of Chemical Physics</i> , 2023, 159, .	3.0	5
976	Gas-phase formation route for <i>trans</i>-HC(O)SH and its isomers under interstellar conditions: a state-of-the-art quantum-chemical study. <i>Monthly Notices of the Royal Astronomical Society</i> , 2023, 525, 1158-1166.	4.4	2
977	Gaâ€Catalyzed Temperatureâ€Dependent Oxazolidinone/Piperazine Synthesis from Phenyl Aziridines Involving a Divergent Ligandâ€Assisted Mechanism. <i>Advanced Synthesis and Catalysis</i> , 2023, 365, 3129-3137.	4.3	2
978	Argon anodic plasma inert anode for Low-Temperature aluminium electrolysis. <i>Chemical Engineering Journal</i> , 2023, 472, 145010.	12.7	1
979	A Systematic Exploration of Bâ€F Bond Dissociation Enthalpies of Fluoroborane-Type Molecules at the CCSD(T)/CBS Level. <i>Molecules</i> , 2023, 28, 5707.	3.8	0
980	Coordination-Promoted Bio-Catechol Electro-Reforming toward Sustainable Polymer Production. <i>Journal of the American Chemical Society</i> , 2023, 145, 18516-18528.	13.7	0
981	Photoisomerisation of Exoâ€imine Complexes and the Role of MECP in the Reverse Thermal Equilibrium: An Experimental and DFT Computational Investigation**. <i>Chemistry - A European Journal</i> , 2023, 29, .	3.3	1
982	One-pot method for in situ synthesis of triple cross-linked hydrogel electrolytes for flexible supercapacitors with high mechanical and electrochemical properties. <i>Journal of Energy Storage</i> , 2023, 72, 108644.	8.1	2

#	ARTICLE	IF	CITATIONS
983	Spectroscopy and Photochemistry of OAINO and Implications for New Metal Chemistry in the Atmosphere. <i>Journal of Physical Chemistry A</i> , 2023, 127, 7618-7629.	2.5	1
984	Benchmarking boron cluster calculations: Establishing reliable geometrical and energetic references for B_n ($n \leq 4$). <i>Journal of Computational Chemistry</i> , 2024, 45, 159-169.	3.9	0
985	Greater transferability and accuracy of norm-conserving pseudopotentials using nonlinear core corrections. <i>Chemical Science</i> , 2023, 14, 10934-10943.	7.4	0
986	High-Field Nonresonant Response of Zundel Cations to Intense Terahertz Radiation. <i>Symmetry</i> , 2023, 15, 1798.	2.2	0
987	Toward Benchmark-Quality <i>Ab Initio</i> Predictions for 3d Transition Metal Electrocatalysts: A Comparison of CCSD(T) and ph-AFQMC. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 6208-6225.	5.3	4
988	The influence of substituents in governing the strength of the $P-X$ bonds of substituted halophosphines R_1R_2P-X ($X = F$ and Cl). <i>Frontiers in Chemistry</i> , 0, 11, .	3.6	0
989	A combined theoretical and experimental study of the pyrolysis of pyrrolidine. <i>Combustion and Flame</i> , 2023, 258, 113063.	5.2	1
990	Investigating the accuracy of density functional methods for molecules in electric fields. <i>Journal of Chemical Physics</i> , 2023, 159, .	3.0	1
991	Theoretical Insights into Midchain Radicals and Branching Characteristics in Solution Copolymerization of Ethylene and Vinyl Acetate. <i>Journal of Physical Chemistry B</i> , 2023, 127, 8268-8281.	2.6	0
992	Liberation of carbon monoxide from formic acid mediated by molybdenum oxyanions. <i>Dalton Transactions</i> , 0, , .	3.3	0
993	Assessment of the nonempirical r2SCAN-QIDH double-hybrid density functional against large and diverse datasets. <i>Journal of Chemical Physics</i> , 2023, 159, .	3.0	3
995	Measurement, correlation, and analysis of the solubility of triethylamine hydrochloride in ten pure solvents. <i>Journal of Molecular Liquids</i> , 2023, 390, 123040.	4.9	1
996	Potential of first row transition metal decorated graphtriyne quantum dots as single atom catalysts towards hydrogen evolution reaction (HER). <i>Physica Scripta</i> , 2023, 98, 115308.	2.5	1
997	Enhancing Stability in Polynitrogen Compounds: Mechanisms and Strategies. <i>Crystal Growth and Design</i> , 0, , .	3.0	0
998	Corrected density functional theory and the random phase approximation: Improved accuracy at little extra cost. <i>Journal of Chemical Physics</i> , 2023, 159, .	3.0	1
999	Non-empirical quadratic-integrand double-hybrid (QIDH) functionals. <i>Annual Reports in Computational Chemistry</i> , 2023, , 87-119.	1.7	0
1000	Design strategy of polyamine for CO ₂ absorption guided by a novel descriptor of hydrogen bond strength. <i>Fuel</i> , 2024, 359, 130393.	6.4	0
1001	Conformational energies of biomolecules in solution: Extending the MPCONF196 benchmark with explicit water molecules. <i>Journal of Computational Chemistry</i> , 2024, 45, 419-429.	3.3	2

#	ARTICLE	IF	CITATIONS
1002	Benchmarking Density Functional Theory Methods for Metalloenzyme Reactions: The Introduction of the MME55 Set. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 8365-8383.	5.3	3
1003	Dispersion-corrected r2SCAN based double-hybrid functionals. <i>Journal of Chemical Physics</i> , 2023, 159, .	3.0	1
1004	Reference Vertical Excitation Energies for Transition Metal Compounds. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 8782-8800.	5.3	0
1005	Noncovalently bound excited-state dimers: a perspective on current time-dependent density functional theory approaches applied to aromatic excimer models. <i>RSC Advances</i> , 2023, 13, 35964-35984.	3.6	1
1006	Redoxâ€chemistry of Pyrimidanes: A DFT Study. <i>European Journal of Inorganic Chemistry</i> , 0, , .	2.0	0
1007	Correlated proton dynamics in hydrogen bonding networks: the benchmark case of 3-hydroxyglutaric acid. <i>Physical Chemistry Chemical Physics</i> , 0, , .	2.8	0
1008	OH Roaming during the Ozonolysis of Î±-Pinene: A New Route to Highly Oxygenated Molecules?. <i>Journal of Physical Chemistry A</i> , 0, , .	2.5	0
1009	Confined Lewis Pairs: Investigation of the X ⁺ Si ₂₀ Interaction in Halogenâ€Encapsulating Silafullerenes. <i>Angewandte Chemie</i> , 2024, 136, .	2.0	0
1010	Confined Lewis Pairs: Investigation of the X ⁺ Si ₂₀ Interaction in Halogenâ€Encapsulating Silafullerenes. <i>Angewandte Chemie - International Edition</i> , 2024, 63, .	13.8	0
1011	LiOtBu-Promoted Intramolecular 1,3-Dipolar Cycloaddition of the 2-alkynyl-biaryl-2-aldehyde N-Tosylhydrazones Approach to 3-Substituted 1H-Dibenzo[e,g]indazoles. <i>Molecules</i> , 2023, 28, 8061.	3.8	0
1012	SOS1-RSX-QIDH: A spin-opposite-scaled range-separated-exchange quadratic-integrand double-hybrid density functional. <i>Journal of Chemical Physics</i> , 2023, 159, .	3.0	0
1013	Influence of Steric and Dispersion Interactions on the Thermochemistry of Crowded (Fluoro)alkyl Compounds. <i>Accounts of Chemical Research</i> , 2024, 57, 153-163.	15.6	1
1014	Exploring CPS-Extrapolated DLPNOâ€CCSD(T ₁) Reference Values for Benchmarking DFT Methods on Enzymatically Catalyzed Reactions. <i>Journal of Physical Chemistry A</i> , 0, , .	2.5	0
1015	Doubling down on density-functional theory. <i>Journal of Chemical Physics</i> , 2023, 159, .	3.0	0
1016	Intramolecular Alkyne-de Mayo Reaction Using the Enol Methylene Acetal Linker: Experimental Implementation and Computational Simulation. <i>Journal of Organic Chemistry</i> , 2024, 89, 939-956.	3.2	0
1017	An Assessment of Dispersion-Corrected DFT Methods for Modeling Nonbonded Interactions in Protein Kinase Inhibitor Complexes. <i>Molecules</i> , 2024, 29, 304.	3.8	0
1018	Enantioselective construction of Si-stereogenic linear alkenylhydrosilanes via copper-catalyzed hydrosilylation of alkynes. <i>Chem Catalysis</i> , 2024, 4, 100887.	6.1	0
1019	Proton affinity Revisited: Benchmarking computational approaches for accurate predictions. <i>Computational and Theoretical Chemistry</i> , 2024, 1233, 114477.	2.5	1

#	ARTICLE	IF	CITATIONS
1020	Regulation of the structure and density of KN ₅ frameworks with CH ₃ COOK and CF ₃ COOK. CrystEngComm, 2024, 26, 951-956.	2.6	0
1021	Molecular interactions of hydrated co-amorphous systems of prilocaine and lidocaine. International Journal of Pharmaceutics, 2024, 651, 123807.	5.2	0
1022	Pyridinium trifluoroacetate ionic liquids as proficient catalysts for synthesis of 3,5,5-trimethyl-2-pyrazoline. ChemistrySelect, 2024, 9, .	1.5	0
1023	Reversible Thiyl Radical Addition~Fragmentation Chain Transfer Polymerization. Angewandte Chemie - International Edition, 2024, 63, .	13.8	0
1024	Reversible Thiyl Radical Addition~Fragmentation Chain Transfer Polymerization. Angewandte Chemie, 2024, 136, .	2.0	0
1025	Separation of Aromatic Hydrocarbons from Straight-Run Naphtha by Bimetallic Halides. Energy & Fuels, 2024, 38, 3262-3274.	5.1	0
1026	Diffusion Monte Carlo method for barrier heights of multiple proton exchanges and complexation energies in small water, ammonia, and hydrogen fluoride clusters. Journal of Chemical Physics, 2024, 160, .	3.0	0
1027	On the General Mechanism for the Gas-phase Reaction of Methanimine with a Radical Species in the Interstellar Medium: Some Failures and an Important Success. Astrophysical Journal, 2024, 962, 32.	4.5	0
1028	Substituent effects on the coordination of benzo-21-crown-7 and dibenzo-21-crown-7 with cesium: Insights from computational chemistry and nuclear magnetic resonance spectroscopy. Journal of Molecular Liquids, 2024, 397, 124169.	4.9	0
1029	Theoretical Prediction of the Reaction Probabilities of H, O, and OH Radicals on the Polypropylene Surface. Journal of Physical Chemistry A, 2024, 128, 1041-1048.	2.5	0
1030	Limiting factors in the accuracy of <sc>DFT</sc> calculation for redox potentials. Journal of Computational Chemistry, 2024, 45, 1177-1186.	3.3	0
1031	Stability and Reactivity of Aromatic Radical Anions in Solution with Relevance to Birch Reduction. Journal of the American Chemical Society, 2024, 146, 8043-8057.	13.7	0
1032	Can astronomical observations be used to constrain crucial chemical reactions? The methoxy case. SOLIS XVIII. Monthly Notices of the Royal Astronomical Society, 2024, 528, 6706-6719.	4.4	0
1033	Enhancing CO ₂ adsorption capacity of hydroxypyridine-based ionic liquids using fluorinated graphene as carrier Material: A density functional theory study. Applied Surface Science, 2024, 659, 159917.	6.1	0
1034	Predicting valence tautomerism in diverse cobalt~dioxolene complexes: elucidation of the role of ligands and solvent. Chemical Science, 2024, 15, 5694-5710.	7.4	0
1035	Using small database and energy descriptors to predict molecular thermodynamic energies through mediated learning models. Chemical Engineering Journal, 2024, 488, 150607.	12.7	0