

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

152 papers	3,576 citations	34 h-index	52 g-index
165 ext. papers	4,247 ext. citations	5.9 avg, IF	6.03 L-index

#	Paper	IF	Citations
152	Effect of structural character of gold nanoparticles in nanofluid on heat pipe thermal performance. <i>Materials Letters</i> , <b>2004</b> , 58, 1461-1465	3.3	274
151	Rapid additive-free selenocystine-selenoester peptide ligation. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 14011-4	16.4	131
150	Controlling charge separation in a novel donor-acceptor metal-organic framework via redox modulation. <i>Chemical Science</i> , <b>2014</b> , 5, 4724-4728	9.4	124
149	G4(MP2)-6X: A Cost-Effective Improvement to G4(MP2). <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 112-20	6.4	119
148	Chemoselective peptide ligation-desulfurization at aspartate. <i>Angewandte Chemie - International Edition</i> , <b>2013</b> , 52, 9723-7	16.4	98
147	Thiosquaramides: pH switchable anion transporters. <i>Chemical Science</i> , <b>2014</b> , 5, 3617-3626	9.4	88
146	Through-Space Intervalence Charge Transfer as a Mechanism for Charge Delocalization in Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 6622-6630	16.4	82
145	W2X and W3X-L: Cost-Effective Approximations to W2 and W4 with kJ mol <sup>-1</sup> Accuracy. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 2109-19	6.4	80
144	Reactivity of disulfide bonds is markedly affected by structure and environment: implications for protein modification and stability. <i>Scientific Reports</i> , <b>2016</b> , 6, 38572	4.9	68
143	Zeolite-catalyzed hydrogenation of carbon dioxide and ethene. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 9790-9	16.4	63
142	W1X-1 and W1X-2: W1-Quality Accuracy with an Order of Magnitude Reduction in Computational Cost. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 4259-69	6.4	59
141	BDE261: a comprehensive set of high-level theoretical bond dissociation enthalpies. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 4975-86	2.8	58
140	Modelling the interaction of molecular hydrogen with lithium-doped hydrogen storage materials. <i>Chemical Physics Letters</i> , <b>2008</b> , 467, 126-130	2.5	57
139	Design of effective zeolite catalysts for the complete hydrogenation of CO <sub>2</sub> . <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 5322-3	16.4	57
138	Obtaining Good Performance With Triple- $\zeta$ -Type Basis Sets in Double-Hybrid Density Functional Theory Procedures. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 2852-63	6.4	52
137	Determination of Barrier Heights for Proton Exchange in Small Water, Ammonia, and Hydrogen Fluoride Clusters with G4(MP2)-Type, MPn, and SCS-MPn Procedures-A Caveat. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 3128-36	6.4	50
136	On the relationship between the preferred site of hydrogen bonding and protonation. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 5509-17	2.8	50

135	Increasing spin crossover cooperativity in 2D Hofmann-type materials with guest molecule removal. <i>Chemical Science</i> , <b>2018</b> , 9, 5623-5629	9.4	50
134	W3X: A Cost-Effective Post-CCSD(T) Composite Procedure. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 4769-78	6.4	47
133	Accelerated Protein Synthesis via One-Pot Ligation-Deselenization Chemistry. <i>CheM</i> , <b>2017</b> , 2, 703-715	16.2	45
132	Assessment of DFT Methods for Transition Metals with the TMC151 Compilation of Data Sets and Comparison with Accuracies for Main-Group Chemistry. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 3610-3622	6.4	45
131	Redox tunable viologen-based porous organic polymers. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 2535-2544	7.5	44
130	Hydrogen abstraction by chlorine atom from amino acids: remarkable influence of polar effects on regioselectivity. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 16553-9	16.4	43
129	Base-catalyzed hydrogenation: rationalizing the effects of catalyst and substrate structures and solvation. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 2443-54	16.4	43
128	Evaluation of the heats of formation of corannulene and C60 by means of high-level theoretical procedures. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 1834-42	2.8	42
127	Hydrogenation of simple aromatic molecules: a computational study of the mechanism. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 924-33	16.4	40
126	Construction of Challenging Proline-Proline Junctions via Diselenide-Selenoester Ligation Chemistry. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 13327-13334	16.4	40
125	Reactivities of amino acid derivatives toward hydrogen abstraction by Cl and OH. <i>Journal of Organic Chemistry</i> , <b>2012</b> , 77, 9807-12	4.2	39
124	Proton-bound homodimers: how are the binding energies related to proton affinities?. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 12197-9	16.4	38
123	Performance of Density Functional Theory Procedures for the Calculation of Proton-Exchange Barriers: Unusual Behavior of M06-Type Functionals. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 3777-83	6.4	37
122	Accurate Computation of Cohesive Energies for Small to Medium-Sized Gold Clusters. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 1964-70	6.4	37
121	A Benchmark Ab Initio and DFT Study of the Structure and Binding of Methane in the $\eta^5$ -Alkane Complex $\text{CpRe}(\text{CO})_2(\text{CH}_4)$ . <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 2199-208	6.4	35
120	Halogenated Metal-Organic Framework Glasses and Liquids. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 3880-3890	16.4	34
119	Assessment of theoretical procedures for hydrogen-atom abstraction by chlorine, and related reactions. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 130, 251-260	1.9	34
118	G4-SP, G4(MP2)-SP, G4-sc, and G4(MP2)-sc: Modifications to G4 and G4(MP2) for the Treatment of Medium-Sized Radicals. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 2647-53	6.4	34

117	Lithium monoxide anion: a ground-state triplet with the strongest base to date. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2008</b> , 105, 7647-51	11.5	34
116	Electronic, optical, and computational studies of a redox-active naphthalenediimide-based coordination polymer. <i>Inorganic Chemistry</i> , <b>2013</b> , 52, 14246-52	5.1	33
115	Factors influencing the formation of polybromide monoanions in solutions of ionic liquid bromide salts. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 7251-60	3.6	32
114	Frequency Scale Factors for Some Double-Hybrid Density Functional Theory Procedures: Accurate Thermochemical Components for High-Level Composite Protocols. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 3774-80	6.4	31
113	Hydrogen-atom abstraction from a model amino acid: dependence on the attacking radical. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 783-8	3.4	29
112	Liquid-phase sintering of lead halide perovskites and metal-organic framework glasses. <i>Science</i> , <b>2021</b> , 374, 621-625	33.3	29
111	Experimental and computational studies of a multi-electron donor-acceptor ligand containing the thiazolo[5,4-d]thiazole core and its incorporation into a metal-organic framework. <i>Chemistry - A European Journal</i> , <b>2014</b> , 20, 17597-605	4.8	27
110	Effect of protonation state and interposed connector groups on bond dissociation enthalpies of alcohols and related systems. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 2810-9	2.8	26
109	Hierarchy of relative bond dissociation enthalpies and their use to efficiently compute accurate absolute bond dissociation enthalpies for C-H, C-C, and C-F bonds. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 3666-75	2.8	26
108	On the inclusion of post-MP2 contributions to double-hybrid density functionals. <i>Journal of Computational Chemistry</i> , <b>2016</b> , 37, 183-93	3.5	25
107	Gas-phase infrared spectrum and acidity of the radical cation of 9-methylguanine. <i>Chemical Communications</i> , <b>2013</b> , 49, 7343-5	5.8	25
106	N-Aryl Groups Are Ubiquitous in Cross-Dehydrogenative Couplings Because They Stabilize Reactive Intermediates. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 9313-9318	4.8	24
105	Approaches for obtaining accurate rate constants for hydrogen abstraction by a chlorine atom. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 3745-52	2.8	24
104	[Fe(C5Ar5)(CO)2Br] complexes as hydrogenase mimics for the catalytic hydrogen evolution reaction. <i>Applied Catalysis B: Environmental</i> , <b>2018</b> , 223, 234-241	21.8	23
103	Bromozincate ionic liquids in the Knoevenagel condensation reaction. <i>Applied Catalysis B: Environmental</i> , <b>2018</b> , 223, 228-233	21.8	23
102	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> , <b>2016</b> , 138, 1420-9	16.4	23
101	Ethylene Trimerisation with Cr-PNP Catalysts: A Theoretical Benchmarking Study and Assessment of Catalyst Oxidation State. <i>Australian Journal of Chemistry</i> , <b>2014</b> , 67, 1481	1.2	22
100	Heats of Formation for CrO, CrO2, and CrO3: An Extreme Challenge for Black-Box Composite Procedures. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 3159-66	6.4	22

99	What factors determine whether a proton-bound homodimer has a symmetric or an asymmetric hydrogen bond?. <i>Molecular Physics</i> , <b>2009</b> , 107, 1095-1105	1.7	22
98	Use of Low-Cost Quantum Chemistry Procedures for Geometry Optimization and Vibrational Frequency Calculations: Determination of Frequency Scale Factors and Application to Reactions of Large Systems. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 6052-6060	6.4	21
97	How to computationally calculate thermochemical properties objectively, accurately, and as economically as possible. <i>Pure and Applied Chemistry</i> , <b>2017</b> , 89, 699-713	2.1	19
96	Toward an Understanding of the Forces Behind Extractive Desulfurization of Fuels with Ionic Liquids. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2019</b> , 7, 4087-4093	8.3	19
95	Heteroatomic deprotonation of substituted methanes and methyl radicals: theoretical insights into structure, stability, and thermochemistry. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 12381-7	2.8	19
94	Chemoselective Peptide LigationDesulfurization at Aspartate. <i>Angewandte Chemie</i> , <b>2013</b> , 125, 9905-9909	3.6	19
93	Probing charge transfer characteristics in a donor-acceptor metal-organic framework by Raman spectroelectrochemistry and pressure-dependence studies. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 25772-25779	3.6	19
92	Accurate quadruple-basis-set approximation for double-hybrid density functional theory with an order of magnitude reduction in computational cost. <i>Theoretical Chemistry Accounts</i> , <b>2014</b> , 133, 1	1.9	18
91	O - H Bond Dissociation Energies. <i>Australian Journal of Chemistry</i> , <b>2011</b> , 64, 394	1.2	18
90	Unification of the W1X and G4(MP2)-6X Composite Protocols. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 2642-2649	6.4	17
89	The electronic, optical and magnetic consequences of delocalization in multifunctional donor-acceptor organic polymers. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 11252-9	3.6	17
88	Synthesis of (+)-luzofuran and (-)-ancistrofuran. <i>Journal of Organic Chemistry</i> , <b>2014</b> , 79, 880-7	4.2	17
87	A Palladium-Catalyzed Multicascade Reaction: Facile Low-Temperature Hydrogenolysis of Activated Nitriles and Related Functional Groups. <i>ChemCatChem</i> , <b>2011</b> , 3, 1496-1502	5.2	17
86	Low barrier hydrogenolysis of the carbon-heteroatom bond as catalyzed by HALF(4). <i>Organic Letters</i> , <b>2009</b> , 11, 749-51	6.2	17
85	Shrinking gold nanoparticles: dramatic effect of a cryogenic process on tannic acid/sodium citrate-generated gold nanoparticles. <i>Materials Letters</i> , <b>2004</b> , 58, 2023-2026	3.3	17
84	Unravelling Some of the Key Transformations in the Hydrothermal Liquefaction of Lignin. <i>ChemSusChem</i> , <b>2017</b> , 10, 2140-2144	8.3	16
83	Outcome-changing effect of polarity reversal in hydrogen-atom-abstraction reactions. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 3843-7	2.8	16
82	Formulation of Small Test Sets Using Large Test Sets for Efficient Assessment of Quantum Chemistry Methods. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 4254-4262	6.4	16

81	Uncatalyzed transfer hydrogenation of quinones and related systems: a theoretical mechanistic study. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 6456-67	2.8	16
80	Understanding Metal-Free Catalytic Hydrogenation: A Systematic Theoretical Study of the Hydrogenation of Ethene. <i>Australian Journal of Chemistry</i> , <b>2004</b> , 57, 659	1.2	16
79	Electrical detection of DNA hybridization with multilayer gold nanoparticles between nanogap electrodes. <i>Microsystem Technologies</i> , <b>2005</b> , 11, 91-96	1.7	16
78	The spectroelectrochemical behaviour of redox-active manganese salen complexes. <i>Dalton Transactions</i> , <b>2019</b> , 48, 3704-3713	4.3	15
77	G4(MP2)-XK: A Variant of the G4(MP2)-6X Composite Method with Expanded Applicability for Main-Group Elements up to Radon. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 4478-4484	6.4	15
76	Watson-Crick Base Pair Radical Cation as a Model for Oxidative Damage in DNA. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 3159-3165	6.4	15
75	A computational study of methanol-to-hydrocarbon conversion ¶Towards the design of a low-barrier process. <i>Canadian Journal of Chemistry</i> , <b>2010</b> , 88, 866-876	0.9	15
74	Hydrogen from Formic Acid via Its Selective Disproportionation over Nanodomain-Modified Zeolites. <i>ACS Catalysis</i> , <b>2015</b> , 5, 4353-4362	13.1	14
73	Preparation of an ion with the highest calculated proton affinity: -diethynylbenzene dianion. <i>Chemical Science</i> , <b>2016</b> , 7, 6245-6250	9.4	14
72	¶Hydrogen Abstraction by ¶H and ¶H Radicals from Amino Acids and Their Peptide Derivatives. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 1606-13	6.4	14
71	¶Bond initiated generation of aryl radicals from aryl diazonium salts. <i>Organic and Biomolecular Chemistry</i> , <b>2020</b> , 18, 1812-1819	3.9	13
70	How accurate are approximate quantum chemical methods at modelling solute-solvent interactions in solvated clusters?. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 3855-3866	3.6	13
69	Effect of Hydrogen Bonding and Partial Deprotonation on the Oxidation of Peptides. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 1741-1746	2.8	13
68	A polar effects controlled enantioselective 1,2-chlorine atom migration via a chlorine-bridged radical intermediate. <i>Journal of the American Chemical Society</i> , <b>2002</b> , 124, 2078-9	16.4	13
67	Gas-phase structure and reactivity of the keto tautomer of the deoxyguanosine radical cation. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 25837-44	3.6	12
66	Performance of Gradient-Corrected and Hybrid Density Functional Theory: Role of the Underlying Local Density Approximation and the Gradient Correction. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 4899-906	6.4	12
65	Structures and thermochemistry of the alkali metal monoxide anions, monoxide radicals, and hydroxides. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 9501-10	2.8	12
64	The CUAGAU Set of Coupled-Cluster Reference Data for Small Copper, Silver, and Gold Compounds and Assessment of DFT Methods. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 5781-5788	2.8	11



63	Restricted-Open-Shell G4(MP2)-Type Procedures. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 9299-9304	2.8	11
62	Transfer hydrogenation between ethane and ethene: a critical assessment of theoretical procedures. <i>Molecular Physics</i> , <b>2006</b> , 104, 777-794	1.7	11
61	Uncatalyzed 1,4-hydrogenation of polycyclic aromatic hydrocarbons: A computational study. <i>Computational and Theoretical Chemistry</i> , <b>2007</b> , 811, 13-17		10
60	Bio-inspired transition metal-organic hydride conjugates for catalysis of transfer hydrogenation: experiment and theory. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 2821-34	4.8	9
59	Excitation energies expressed as orbital energies of Kohn-Sham density functional theory with long-range corrected functionals. <i>Journal of Computational Chemistry</i> , <b>2020</b> , 41, 1368-1383	3.5	9
58	Hydrogen from formic acid through its selective disproportionation over sodium germanate--a non-transition-metal catalysis system. <i>Angewandte Chemie - International Edition</i> , <b>2014</b> , 53, 11275-9	16.4	9
57	Correlation functional in screened-exchange density functional theory procedures. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 2307-2315	3.5	9
56	Role of Hydrogen Bonding on the Reactivity of Thiyl Radicals: A Mass Spectrometric and Computational Study Using the Distonic Radical Ion Approach. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 8184-8189	2.8	9
55	Aqueous-Phase Conformations of Lactose, Maltose, and Sucrose and the Assessment of Low-Cost DFT Methods with the DSCONF Set of Conformers for the Three Disaccharides. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 582-590	2.8	8
54	Beyond the Halogen Bond: Examining the Limits of Extended Polybromide Networks through Quantum-Chemical Investigations. <i>Chemistry - an Asian Journal</i> , <b>2016</b> , 11, 682-6	4.5	8
53	Hydrogen-atom attack on phenol and toluene is ortho-directed. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 8625-36	3.6	8
52	Gas-phase synthesis and reactivity of lithium acetylide ion, Li-C[triple bond]C-. <i>Angewandte Chemie - International Edition</i> , <b>2010</b> , 49, 5161-4	16.4	8
51	Assessment and development of DFT with the expanded CUAGAU-2 set of group-11 cluster systems. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26453	2.1	8
50	Applications of isodesmic-type reactions for computational thermochemistry. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2021</b> , 11, e1501	7.9	8
49	A Simple Model for Relative Energies of All Fullerenes Reveals the Interplay between Intrinsic Resonance and Structural Deformation Effects in Medium-Sized Fullerenes. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 1255-1264	6.4	7
48	Accurate Thermochemical and Kinetic Stabilities of C Isomers. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 4768-4777	2.8	7
47	Interligand Charge-Transfer Interactions in Electroactive Coordination Frameworks Based on N, NRDicyanoquinonediimine (DCNQI). <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 9766-9774	5.1	7
46	Charge-Transfer Excitation Energies Expressed as Orbital Energies of Kohn-Sham Density Functional Theory with Long-Range Corrected Functionals. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 8079-8087	2.8	7

45	Spectroscopic, electronic and computational properties of a mixed tetrachalcogenafulvalene and its charge transfer complex. <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 1092-1104	7.1	7
44	Impact of Hydrogen Bonding on the Susceptibility of Peptides to Oxidation. <i>Chemistry - an Asian Journal</i> , <b>2017</b> , 12, 1485-1489	4.5	6
43	H and D attachment to naphthalene: spectra and thermochemistry of cold gas-phase 1-C10H9 and 1-C10H8D radicals and cations. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 3225-32	2.8	6
42	Toward the complete range separation of non-hybrid exchange-correlation functional. <i>Journal of Computational Chemistry</i> , <b>2015</b> , 36, 871-7	3.5	6
41	Ni-Catalyzed Formal Carbonyl-Ene Reaction of Terminal Alkenes via Carbon Dioxide Insertion. <i>Synlett</i> , <b>2018</b> , 29, 742-746	2.2	6
40	Rapid Prediction of Ultraviolet-Visible Spectra from Conventional (Non-Time-Dependent) Density Functional Theory Calculations. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 7882-7885	6.4	6
39	Fullerene Thermochemical Stability: Accurate Heats of Formation for Small Fullerenes, the Importance of Structural Deformation on Reactivity, and the Special Stability of C. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 6688-6698	2.8	6
38	Barriometry - an enhanced database of accurate barrier heights for gas-phase reactions. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 10732-10740	3.6	5
37	KoopmansRTYPE Theorem in Kohn-Sham Theory with Optimally Tuned Long-Range-Corrected (LC) Functionals. <i>Journal of Physical Chemistry A</i> , <b>2021</b> , 125, 3489-3502	2.8	5
36	Performance of the OP correlation functional in relation to its formulation: Influence of the exchange component and the effect of incorporating same-spin correlations. <i>Journal of Computational Chemistry</i> , <b>2016</b> , 37, 1306-12	3.5	5
35	The reHISS Three-Range Exchange Functional with an Optimal Variation of Hartree-Fock and Its Use in the reHISSB-D Density Functional Theory Method. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 29-38	3.5	5
34	A cofacial metal-organic framework based photocathode for carbon dioxide reduction. <i>Chemical Science</i> , <b>2021</b> , 12, 3608-3614	9.4	5
33	A redox-active ionic liquid manifesting charge-transfer interaction between a viologen and carbazole and its effect on the viscosity, ionic conductivity, and redox process of the viologen. <i>Chemical Science</i> , <b>2021</b> , 12, 4872-4882	9.4	5
32	Mechanism for Three-Component Ni-Catalyzed Carbonyl-Ene Reaction for CO <sub>2</sub> Transformation: What Practical Lessons Do We Learn from DFT Modelling?. <i>Australian Journal of Chemistry</i> , <b>2018</b> , 71, 272	1.2	5
31	Core-Level Excitation Energies of Nucleic Acid Bases Expressed as Orbital Energies of the Kohn-Sham Density Functional Theory with Long-Range Corrected Functionals. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 10482-10494	2.8	4
30	Hydrothermal Liquefaction of EO-4 Aryl Ether Linkages in Lignin. <i>ChemSusChem</i> , <b>2020</b> , 13, 2002-2006	8.3	4
29	Modelling the Effect of Conformation on Hydrogen-Atom Abstraction from Peptides. <i>Australian Journal of Chemistry</i> , <b>2018</b> , 71, 257	1.2	4
28	Hydrogen-adduction to open-shell graphene fragments: spectroscopy, thermochemistry and astrochemistry. <i>Chemical Science</i> , <b>2017</b> , 8, 1186-1194	9.4	4



27	An ONIOM investigation of the effect of conformation on bond dissociation energies in peptides. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 82-88	3.5	4
26	Thermochemical stabilities of giant fullerenes using density functional tight binding theory and isodesmic-type reactions. <i>Journal of Computational Chemistry</i> , <b>2021</b> , 42, 222-230	3.5	4
25	Proton-bound homodimers involving second-row atoms. <i>Theoretical Chemistry Accounts</i> , <b>2012</b> , 131, 1	1.9	3
24	Comment on the ionization energy of B <sub>2</sub> F <sub>4</sub> . <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 9214-5	2.8	3
23	The outcome of the oxidations of unusual enediamide motifs is governed by the stabilities of the intermediate iminium ions. <i>PLoS ONE</i> , <b>2012</b> , 7, e47224	3.7	3
22	Benchmark study of DFT and composite methods for bond dissociation energies in argon compounds. <i>Chemical Physics</i> , <b>2020</b> , 531, 110676	2.3	3
21	An improved Slater's transition state approximation. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 034101	3.9	3
20	Hydrogen from Formic Acid through Its Selective Disproportionation over Sodium Germanate: A Non-Transition-Metal Catalysis System. <i>Angewandte Chemie</i> , <b>2014</b> , 126, 11457-11461	3.6	2
19	Stereoselective radical bromination of $\alpha$ -chloro hydrocinnamic acid derivatives. <i>Tetrahedron Letters</i> , <b>2000</b> , 41, 2671-2674	2	2
18	Accurate Quantum Chemical Prediction of Gas-Phase Anion Binding Affinities and Their Structure-Binding Relationships. <i>Journal of Physical Chemistry A</i> , <b>2021</b> , 125, 9838-9851	2.8	2
17	Fluorination effect on electrochemistry of dibutyl viologen in aqueous solution. <i>Journal of Electroanalytical Chemistry</i> , <b>2020</b> , 856, 113691	4.1	2
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15	Gas-Phase Synthesis and Reactivity of Lithium Acetylide Ion, LiC <sub>2</sub> C <sup>-</sup> . <i>Angewandte Chemie</i> , <b>2010</b> , 122, 5287-5290	3.6	1
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11	Hydride Affinities for Main-Group Hydride Reductants: Assessment of Density Functionals and Trends in Reactivities. <i>Journal of Physical Chemistry A</i> , <b>2021</b> , 125, 835-842	2.8	1
10	Higher-order transition state approximation.. <i>Journal of Chemical Physics</i> , <b>2022</b> , 156, 114112	3.9	1

9	Methylation with Dimethyl Carbonate/Dimethyl Sulfide Mixtures: An Integrated Process without Addition of Acid/Base and Formation of Residual Salts.. <i>ChemSusChem</i> , <b>2021</b> , e202102538	8.3	1
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6	Substituent effects on through-space intervalence charge transfer in cofacial metal-organic frameworks. <i>Faraday Discussions</i> , <b>2021</b> , 231, 152-167	3.6	0
5	Polycyclic aromatic hydrocarbons: from small molecules through nano-sized species towards bulk graphene. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 17713-17723	3.6	0
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