Amir Karton

List of Publications by Citations

179 papers	6,816 citations	44 h-index	78 g-index
189 ext. papers	7,830 ext. citations	4.4 avg, IF	6.68 L-index

#	Paper	IF	Citations
179	Highly accurate first-principles benchmark data sets for the parametrization and validation of density functional and other approximate methods. Derivation of a robust, generally applicable, double-hybrid functional for thermochemistry and thermochemical kinetics. *Journal of Physical Chemistry A*, **2008**, 112, 12868-86	2.8	578
178	W4 theory for computational thermochemistry: In pursuit of confident sub-kJ/mol predictions. *Journal of Chemical Physics*, **2006**, 125, 144108	3.9	561
177	Comment on: Estimating the Hartree–Fock limit from finite basis set calculations [Jensen F (2005) Theor Chem Acc 113:267]. *Theoretical Chemistry Accounts*, **2006**, 115, 330-333	1.9	318
176	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. *Chemical Physics Letters*, **2011**, 510, 165-178	2.5	285
175	Double-hybrid functionals for thermochemical kinetics. *Journal of Physical Chemistry A*, **2008**, 112, 3-8	2.8	194
174	Benchmark study of DFT functionals for late-transition-metal reactions. *Journal of Physical Chemistry A*, **2006**, 110, 709-16	2.8	193
173	Explicitly correlated Wn theory: W1-F12 and W2-F12. *Journal of Chemical Physics*, **2012**, 136, 124114	3.9	176
172	A computational chemist's guide to accurate thermochemistry for organic molecules. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 292-310	7.9	137
171	Performance of ab initio and density functional methods for conformational equilibria of C(n)H(2n+2) alkane isomers (n = 4-8). *Journal of Physical Chemistry A*, **2009**, 113, 11974-83	2.8	134
170	Bioinspired graphene membrane with temperature tunable channels for water gating and molecular separation. *Nature Communications*, **2017**, 8, 2011	17.4	130
169	Basis set convergence of post-CCSD contributions to molecular atomization energies. *Journal of Chemical Physics*, **2007**, 127, 064104	3.9	127
168	Benchmark thermochemistry of the C(n)H(2n+2) alkane isomers (n = 2-8) and performance of DFT and composite ab initio methods for dispersion-driven isomeric equilibria. *Journal of Physical Chemistry A*, **2009**, 113, 8434-47	2.8	110
167	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, 622-32	3.5	92
166	Model for the exceptional reactivity of peroxiredoxins 2 and 3 with hydrogen peroxide: a kinetic and computational study. *Journal of Biological Chemistry*, **2011**, 286, 18048-55	5.4	92
165	Proton enhanced dynamic battery chemistry for aprotic lithium-oxygen batteries. *Nature Communications*, **2017**, 8, 14308	17.4	88
164	A simple DFT-based diagnostic for nondynamical correlation. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	88
163	W4-17: A diverse and high-confidence dataset of atomization energies for benchmarking high-level electronic structure methods. *Journal of Computational Chemistry*, **2017**, 38, 2063-2075	3.5	85

162	Heats of formation of beryllium, boron, aluminum, and silicon re-examined by means of W4 theory. *Journal of Physical Chemistry A*, **2007**, 111, 5936-44	2.8	82
161	Co-Crystallization of Sym-Triiodo-Trifluorobenzene with Bipyridyl Donors: Consistent Formation of Two Instead of Anticipated Three N···I Halogen Bonds. *Crystal Growth and Design*, **2007**, 7, 386-392	3.5	81
160	The melatonin conformer space: benchmark and assessment of wave function and DFT methods for a paradigmatic biological and pharmacological molecule. *Journal of Physical Chemistry A*, **2013**, 117, 2269-77	2.8	77
159	Benchmark ab Initio Conformational Energies for the Proteinogenic Amino Acids through Explicitly Correlated Methods. Assessment of Density Functional Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 444-54	6.4	75
158	Post-CCSD(T) ab initio thermochemistry of halogen oxides and related hydrides XOX, XOOX, HOX, XOn, and HXOn (X = F, Cl), and evaluation of DFT methods for these systems. *Journal of Physical Chemistry A*, **2009**, 113, 4802-16	2.8	71
157	Toward a W4-F12 approach: Can explicitly correlated and orbital-based ab initio CCSD(T) limits be reconciled?. *Journal of Chemical Physics*, **2016**, 144, 214101	3.9	69
156	Blue phosphorene monolayers as potential nano sensors for volatile organic compounds under point defects. *Applied Surface Science*, **2019**, 486, 52-57	6.7	68
155	Assessment of theoretical procedures for calculating barrier heights for a diverse set of water-catalyzed proton-transfer reactions. *Journal of Physical Chemistry A*, **2012**, 116, 4211-21	2.8	65
154	Stable room-temperature molecular negative differential resistance based on molecule-electrode interface chemistry. *Journal of the American Chemical Society*, **2004**, 126, 11648-57	16.4	65
153	Borane-lewis base complexes as homolytic hydrogen atom donors. *Chemistry - A European Journal*, **2010**, 16, 6861-5	4.8	64
152	Heats of formation of the amino acids re-examined by means of W1-F12 and W2-F12 theories. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	63
151	Selective sp3 C-H activation of ketones at the beta position by Ir(I). Origin of regioselectivity and water effect. *Journal of the American Chemical Society*, **2006**, 128, 12400-1	16.4	63
150	Directing aryl-I versus Aryl-Br bond activation by nickel via a ring walking process. *Inorganic Chemistry*, **2008**, 47, 5114-21	5.1	60
149	Enhancement in hydrogen storage capacities of light metal functionalized Boron□raphdiyne nanosheets. *Carbon*, **2019**, 147, 199-205	10.4	59
148	Accurate quantum chemical energies for tetrapeptide conformations: why MP2 data with an insufficient basis set should be handled with caution. *Physical Chemistry Chemical Physics*, **2013**, 15, 7028-31	3.6	57
147	Benchmark atomization energy of ethane: Importance of accurate zero-point vibrational energies and diagonal Born□ppenheimer corrections for a □imple□rganic molecule. *Computational and Theoretical Chemistry*, **2007**, 811, 345-353		57
146	Performance of W4 theory for spectroscopic constants and electrical properties of small molecules. *Journal of Chemical Physics*, **2010**, 133, 144102	3.9	56
145	Economical post-CCSD(T) computational thermochemistry protocol and applications to some aromatic compounds. *Journal of Physical Chemistry A*, **2009**, 113, 7610-20	2.8	55

144	Platinum stilbazoles: ring-walking coupled with aryl-halide bond activation. *Journal of the American Chemical Society*, **2005**, 127, 9322-3	16.4	54
143	Reaction barrier heights for cycloreversion of heterocyclic rings: An Achilles heel for DFT and standard ab initio procedures. *Chemical Physics*, **2015**, 458, 1-8	2.3	51
142	Inorganic acid-catalyzed tautomerization of vinyl alcohol to acetaldehyde. *Chemical Physics Letters*, **2014**, 592, 330-333	2.5	50
141	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. *Journal of Chemical Theory and Computation*, **2012**, 8, 3128-36	6.4	50
140	Heats of formation of platonic hydrocarbon cages by means of high-level thermochemical procedures. *Journal of Computational Chemistry*, **2016**, 37, 49-58	3.5	47
139	Explicitly correlated benchmark calculations on C8H8 isomer energy separations: how accurate are DFT, double-hybrid, and composite ab initio procedures?. *Molecular Physics*, **2012**, 110, 2477-2491	1.7	47
138	Efficient and selective sensing of nitrogen-containing gases by Si2BN nanosheets under pristine and pre-oxidized conditions. *Applied Surface Science*, **2019**, 469, 775-780	6.7	47
137	Potassium Poly(Heptazine Imide): Transition Metal-Free Solid-State Triplet Sensitizer in Cascade Energy Transfer and [3+2]-cycloadditions. *Angewandte Chemie - International Edition*, **2020**, 59, 15061-15068	16.4	46
136	Heterologous biosynthesis of elsinochrome A sheds light on the formation of the photosensitive perylenequinone system. *Chemical Science*, **2019**, 10, 1457-1465	9.4	44
135	Thermoresponsive Graphene Membranes with Reversible Gating Regularity for Smart Fluid Control. *Advanced Functional Materials*, **2019**, 29, 1808501	15.6	43
134	NLO properties of metallabenzene-based chromophores: a time-dependent density functional study. *Journal of Physical Chemistry A*, **2005**, 109, 5454-62	2.8	43
133	Remarkable improvement in hydrogen storage capacities of two-dimensional carbon nitride (g-C3N4) nanosheets under selected transition metal doping. *International Journal of Hydrogen Energy*, **2020**, 45, 3035-3045	6.7	43
132	Elemental Substitution of Two-Dimensional Transition Metal Dichalcogenides (MoSe and MoTe): Implications for Enhanced Gas Sensing. *ACS Sensors*, **2019**, 4, 2646-2653	9.2	42
131	Evaluation of the heats of formation of corannulene and C60 by means of high-level theoretical procedures. *Journal of Physical Chemistry A*, **2013**, 117, 1834-42	2.8	42
130	Drastic Improvement in Gas-Sensing Characteristics of Phosphorene Nanosheets under Vacancy Defects and Elemental Functionalization. *Journal of Physical Chemistry C*, **2018**, 122, 20186-20193	3.8	41
129	Assessment of theoretical procedures for a diverse set of isomerization reactions involving double-bond migration in conjugated dienes. *Chemical Physics*, **2014**, 441, 166-177	2.3	39
128	The lowest singlet-triplet excitation energy of BN: A converged coupled cluster perspective. *Journal of Chemical Physics*, **2006**, 125, 144313	3.9	39
127	Sensing of volatile organic compounds on two-dimensional nitrogenated holey graphene, graphdiyne, and their heterostructure. *Carbon*, **2020**, 163, 213-223	10.4	38

126	Basis set convergence of CCSD(T) equilibrium geometries using a large and diverse set of molecular structures. *Journal of Chemical Physics*, **2016**, 145, 104101	3.9	38
125	Reversible hydrogen storage properties of defect-engineered C4N nanosheets under ambient conditions. *Carbon*, **2019**, 152, 344-353	10.4	37
124	Chemically induced repair, adhesion, and recycling of polymers made by inverse vulcanization. *Chemical Science*, **2020**, 11, 5537-5546	9.4	37
123	Sol-Gel auto-combustion synthesis and physicochemical properties of BaAl2O4 nanoparticles; electrochemical hydrogen storage performance and density functional theory. *Renewable Energy*, **2017**, 114, 1419-1426	8.1	37
122	N?H and N?Cl homolytic bond dissociation energies and radical stabilization energies: An assessment of theoretical procedures through comparison with benchmark-quality W2w data. *International Journal of Quantum Chemistry*, **2012**, 112, 1862-1878	2.1	37
121	Atomization energies of the carbon clusters C n (n = 2–10) revisited by means of W4 theory as well as density functional, Gn, and CBS methods. *Molecular Physics*, **2009**, 107, 977-990	1.7	37
120	Real-time 2D NMR identification of analytes undergoing continuous chromatographic separation. *Journal of the American Chemical Society*, **2004**, 126, 1262-5	16.4	35
119	Pinning the most stable HxCyOz isomers in space by means of high-level theoretical procedures. *Chemical Physics*, **2014**, 436-437, 22-28	2.3	32
118	Novel green phosphorene as a superior chemical gas sensing material. *Journal of Hazardous Materials*, **2021**, 401, 123340	12.8	32
117	The S66 Non-Covalent Interactions Benchmark Reconsidered Using Explicitly Correlated Methods Near the Basis Set Limit. *Australian Journal of Chemistry*, **2018**, 71, 238	1.2	30
116	Reactive Compression Molding Post-Inverse Vulcanization: A Method to Assemble, Recycle, and Repurpose Sulfur Polymers and Composites. *Chemistry - A European Journal*, **2020**, 26, 10035-10044	4.8	29
115	Covalency and Ionicity Do Not Oppose Each Other-Relationship Between Si-O Bond Character and Basicity of Siloxanes. *Chemistry - A European Journal*, **2018**, 24, 15275-15286	4.8	28
114	Dy3Al2(AlO4)3 ceramic nanogarnets: Sol-gel auto-combustion synthesis, characterization and joint experimental and computational structural analysis for electrochemical hydrogen storage performances. *Journal of Alloys and Compounds*, **2018**, 744, 574-582	5.7	26
113	Study of dual encapsulation possibility of hydrophobic and hydrophilic drugs into a nanocarrier based on bio-polymer coated graphene oxide using density functional theory, molecular dynamics simulation and experimental methods. *Journal of Molecular Liquids*, **2018**, 262, 204-217	6	26
112	Effect of substituents on the strength of N-X (X = H, F, and Cl) bond dissociation energies: a high-level quantum chemical study. *Journal of Physical Chemistry A*, **2011**, 115, 5496-504	2.8	26
111	Graphitic carbon nitride nano sheets functionalized with selected transition metal dopants: an efficient way to store CO. *Nanotechnology*, **2018**, 29, 415502	3.4	23
110	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	3.5	23
109	Basis set convergence of explicitly correlated double-hybrid density functional theory calculations. *Journal of Chemical Physics*, **2011**, 135, 144119	3.9	23

108	Metal functionalized inorganic nano-sheets as promising materials for clean energy storage. *Applied Surface Science*, **2019**, 471, 887-892	6.7	23
107	Tailoring the capability of carbon nitride (CN) nanosheets toward hydrogen storage upon light transition metal decoration. *Nanotechnology*, **2019**, 30, 075404	3.4	23
106	From High-Energy CH Isomers with A Planar Tetracoordinate Carbon Atom to An Experimentally Known Carbene. *Journal of Physical Chemistry A*, **2018**, 122, 9054-9064	2.8	23
105	Heats of Formation for CrO, CrO2, and CrO3: An Extreme Challenge for Black-Box Composite Procedures. *Journal of Chemical Theory and Computation*, **2012**, 8, 3159-66	6.4	22
104	A dataset of highly accurate homolytic N?Br bond dissociation energies obtained by Means of W2 theory. *International Journal of Quantum Chemistry*, **2016**, 116, 52-60	2.1	22
103	Effect of substituents on the preferred modes of one-electron reductive cleavage of N-Cl and N-Br bonds. *Journal of Physical Chemistry A*, **2013**, 117, 460-72	2.8	20
102	Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. *Molecular Physics*, **2016**, 114, 21-33	1.7	18
101	Highly Accurate CCSDT(Q)/CBS Reaction Barrier Heights for a Diverse Set of Transition Structures: Basis Set Convergence and Cost-Effective Approaches for Estimating Post-CCSD(T) Contributions. *Journal of Physical Chemistry A*, **2019**, 123, 6720-6732	2.8	18
100	The adsorption and migration behavior of divalent metals (Mg, Ca, and Zn) on pristine and defective graphene. *Carbon*, **2020**, 163, 276-287	10.4	17
99	Functionalized Two-Dimensional Nanoporous Graphene as Efficient Global Anode Materials for Li-, Na-, K-, Mg-, and Ca-Ion Batteries. *Journal of Physical Chemistry C*, **2020**, 124, 9734-9745	3.8	17
98	An assessment of theoretical procedures for □conjugation stabilisation energies in enones. *Molecular Physics*, **2015**, 113, 1284-1296	1.7	16
97	Bond orders for intermolecular interactions in crystals: charge transfer, ionicity and the effect on intramolecular bonds. *IUCrJ*, **2018**, 5, 635-646	4.7	16
96	[Al2O4](-), a Benchmark Gas-Phase Class II Mixed-Valence Radical Anion for the Evaluation of Quantum-Chemical Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 3796-806	6.4	15
95	G4(MP2)-XK: A Variant of the G4(MP2)-6X Composite Method with Expanded Applicability for Main-Group Elements up to Radon. *Journal of Chemical Theory and Computation*, **2019**, 15, 4478-4484	6.4	15
94	Inversion and rotation processes involving non-planar aromatic compounds catalyzed by extended polycyclic aromatic hydrocarbons. *Chemical Physics Letters*, **2014**, 614, 156-161	2.5	15
93	O(3P) + CO2 collisions at hyperthermal energies: dynamics of nonreactive scattering, oxygen isotope exchange, and oxygen-atom abstraction. *Journal of Physical Chemistry A*, **2012**, 116, 64-84	2.8	15
92	Computational design of effective, bioinspired HOCl antioxidants: the role of intramolecular Cl+ and H+ shifts. *Journal of the American Chemical Society*, **2012**, 134, 19240-5	16.4	15
91	Toward Improved Performance of All-Organic Nitroxide Radical Batteries with Ionic Liquids: A Theoretical Perspective. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 5367-5375	8.3	14

90	Hydrogen Abstraction by OH and SH Radicals from Amino Acids and Their Peptide Derivatives. *Journal of Chemical Theory and Computation*, **2016**, 12, 1606-13	6.4	14
89	Heat of formation for C 60 by means of the G4(MP2) thermochemical protocol through reactions in which C 60 is broken down into corannulene and sumanene. *Chemical Physics Letters*, **2016**, 643, 34-38	2.5	14
88	Post-CCSD(T) contributions to total atomization energies in multireference systems. *Journal of Chemical Physics*, **2018**, 149, 034102	3.9	14
87	W4 thermochemistry of P2 and P4. Is the CODATA heat of formation of the phosphorus atom correct?. *Molecular Physics*, **2007**, 105, 2499-2505	1.7	14
86	Evaluation of density functional theory for a large and diverse set of organic and inorganic equilibrium structures. *Journal of Computational Chemistry*, **2021**, 42, 1590-1601	3.5	14
85	The High Performance of Choline Arginate for Biomass Pretreatment Is Due to Remarkably Strong Hydrogen Bonding by the Anion. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 4115-4121	8.3	13
84	Energetic and spectroscopic properties of the low-lying CH isomers: a high-level ab initio perspective. *Physical Chemistry Chemical Physics*, **2017**, 19, 17685-17697	3.6	13
83	Theoretical Studies of SiCH Isomers Delineate Three Low-Lying Silylidenes Are Missing in the Laboratory. *Journal of Physical Chemistry A*, **2020**, 124, 987-1002	2.8	13
82	Mechanistic Insights into Water-Catalyzed Formation of Levoglucosenone from Anhydrosugar Intermediates by Means of High-Level Theoretical Procedures. *Australian Journal of Chemistry*, **2016**, 69, 943	1.2	13
81	Performance of DFT for C Isomerization Energies: A Noticeable Exception to Jacob's Ladder. *Journal of Physical Chemistry A*, **2019**, 123, 257-266	2.8	13
80	How large are post-CCSD(T) contributions to the total atomization energies of medium-sized alkanes?. *Chemical Physics Letters*, **2016**, 645, 118-122	2.5	12
79	MVO-10: A Gas-Phase Oxide Benchmark for Localization/Delocalization in Mixed-Valence Systems. *Journal of Chemical Theory and Computation*, **2018**, 14, 3512-3523	6.4	12
78	A coordination controlled aryl-halide oxidative addition to platinum. *Chemistry - A European Journal* , **2009**, 15, 10025-8	4.8	12
77	Comment on "Revised electron affinity of SF6 from kinetic data" [J. Chem. Phys. 136, 121102 (2012)]. *Journal of Chemical Physics*, **2012**, 136, 197101	3.9	12
76	Restricted-Open-Shell G4(MP2)-Type Procedures. *Journal of Physical Chemistry A*, **2016**, 120, 9299-9304	2.8	11
75	Parapheromones for Thynnine Wasps. *Journal of Chemical Ecology*, **2016**, 42, 17-23	2.7	11
74	Basis set convergence of high-order coupled cluster methods up to CCSDTQ567 for a highly multireference molecule. *Chemical Physics Letters*, **2019**, 737, 136810	2.5	11
73	Sneaking up on the Criegee intermediate from below: Predicted photoelectron spectrum of the CH_2OO^- anion and W3-F12 electron affinity of CH_2OO. *Chemical Physics Letters*, **2013**, 585, 15-20	2.5	11

72	Computational investigation into the gas-phase ozonolysis of the conjugated monoterpene □phellandrene. *Physical Chemistry Chemical Physics*, **2016**, 18, 27991-28002	3.6	11
71	Sensitivity enhancement of stanene towards toxic SO2 and H2S. *Applied Surface Science*, **2019**, 495, 143622	6.7	10
70	Catalysis by Pure Graphene-From Supporting Actor to Protagonist through Shape Complementarity. *Journal of Organic Chemistry*, **2019**, 84, 11343-11347	4.2	10
69	Theoretical Studies of Two Key Low-Lying Carbenes of CH Missing in the Laboratory. *Journal of Physical Chemistry A*, **2019**, 123, 6618-6627	2.8	10
68	Estimating the CCSD basis-set limit energy from small basis sets: basis-set extrapolations vs additivity schemes. *AIP Advances*, **2015**, 5, 057148	1.5	10
67	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	3.5	10
66	An extended N-H bond, driven by a conserved second-order interaction, orients the flavin N5 orbital in cholesterol oxidase. *Scientific Reports*, **2017**, 7, 40517	4.9	9
65	Kalium-Polyheptazinimid: Ein □bergangsmetallfreier Festk□per-Triplett-Sensibilisator in Kaskadenenergietransfer und [3+2]-Cycloadditionen. *Angewandte Chemie*, **2020**, 132, 15172-15180	3.6	9
64	Predicting the primary fragments in mass spectrometry using ab initio Roby□ould bond indices. *International Journal of Quantum Chemistry*, **2018**, 118, e25603	2.1	9
63	Computational insights for the hydride transfer and distinctive roles of key residues in cholesterol oxidase. *Scientific Reports*, **2017**, 7, 17265	4.9	9
62	Manganese-Catalyzed Hydroboration of Terminal Olefins and Metal-Dependent Selectivity in Internal Olefin Isomerization-Hydroboration. *Inorganic Chemistry*, **2021**, 60, 494-504	5.1	9
61	Quantum chemical electron impact mass spectrum prediction for de novo structure elucidation: Assessment against experimental reference data and comparison to competitive fragmentation modeling. *International Journal of Quantum Chemistry*, **2018**, 118, e25460	2.1	8
60	Evaluation of the performance of MP4-based procedures for a wide range of thermochemical and kinetic properties. *Chemical Physics*, **2016**, 480, 23-35	2.3	8
59	High-resolution structures of cholesterol oxidase in the reduced state provide insights into redox stabilization. *Acta Crystallographica Section D: Biological Crystallography*, **2014**, 70, 3155-66		8
58	The quest for the carbene bent-pentadiynylidene isomer of C5H2. *Chemical Physics*, **2018**, 515, 411-417	2.3	8
57	Pristine Graphene as a Racemization Catalyst for Axially Chiral BINOL. *ChemPhysChem*, **2020**, 21, 1675-1681	3.2	7
56	Accurate Thermochemical and Kinetic Stabilities of C Isomers. *Journal of Physical Chemistry A*, **2018**, 122, 4768-4777	2.8	7
55	Structure-Activity Studies of Semiochemicals from the Spider Orchid Caladenia plicata for Sexual Deception. *Journal of Chemical Ecology*, **2018**, 44, 436-443	2.7	7

54	Carnosine and Carcinine Derivatives Rapidly React with Hypochlorous Acid to Form Chloramines and Dichloramines. *Chemical Research in Toxicology*, **2019**, 32, 513-525	4	6
53	Investigation of an Unusual Crystal Habit of Hydrochlorothiazide Reveals Large Polar Enantiopure Domains and a Possible Crystal Nucleation Mechanism. *Angewandte Chemie - International Edition*, **2019**, 58, 10255-10259	16.4	6
52	A computational investigation of the sulphuric acid-catalysed 1,4-hydrogen transfer in higher Criegee intermediates. *International Journal of Quantum Chemistry*, **2018**, 118, e25599	2.1	6
51	Effective basis set extrapolations for CCSDT, CCSDT(Q), and CCSDTQ correlation energies. *Journal of Chemical Physics*, **2020**, 153, 024102	3.9	6
50	Catalysis on Pristine 2D Materials via Dispersion and Electrostatic Interactions. *Journal of Physical Chemistry A*, **2020**, 124, 6977-6985	2.8	6
49	Can force fields developed for carbon nanomaterials describe the isomerization energies of fullerenes?. *Chemical Physics Letters*, **2021**, 779, 138853	2.5	6
48	Quantum mechanical tunnelling: the missing term to achieve sub-kJ mol barrier heights. *Physical Chemistry Chemical Physics*, **2021**, 23, 10888-10898	3.6	6
47	Sulphuric acid-catalysed formation of hemiacetal from glyoxal and ethanol. *Chemical Physics Letters* , **2017**, 675, 27-34	2.5	5
46	Deciphering the exceptional selectivity of semipinacol rearrangements in cis-fused □-lactam diols using high-level quantum chemical methods. *Organic Chemistry Frontiers*, **2019**, 6, 725-731	5.2	5
45	Spontaneous shape and phase control of colloidal ZnSe nanocrystals by tailoring Se precursor reactivity. *CrystEngComm*, **2019**, 21, 2955-2961	3.3	5
44	The CH3CHOO □riegee intermediate□and its anion: Isomers, infrared spectra, and W3-F12 energetics. *Chemical Physics Letters*, **2015**, 621, 193-198	2.5	5
43	Moir□patterns arising from bilayer graphone/graphene superlattice. *Nano Research*, **2020**, 13, 1060-1064	10	5
42	Can Popular DFT Approximations and Truncated Coupled Cluster Theory Describe the Potential Energy Surface of the Beryllium Dimer?. *Australian Journal of Chemistry*, **2018**, 71, 804	1.2	5
41	Computational design of bio-inspired carnosine-based HOBr antioxidants. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 905-913	4.2	5
40	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	2.1	5
39	The reaction of the benzene cation with acetylenes for the growth of PAHs in the interstellar medium. *Chemical Physics Letters*, **2014**, 595-596, 13-19	2.5	5
38	To bridge or not to bridge: The role of sulfuric acid in the Beckmann rearrangement. *Chemical Physics Letters*, **2016**, 659, 100-104	2.5	5
37	Can density functional theory □ope□with highly fluxional shapeshifting molecules?. *Chemical Physics*, **2021**, 540, 111013	2.3	5

36	Experimental and Theoretical Study of the Chemical Network of the Hydrogenation of NO on Interstellar Dust Grains. *ACS Earth and Space Chemistry*, **2019**, 3, 1196-1207	3.2	4
35	A Computational Investigation of the Uncatalysed and Water-Catalysed Acyl Rearrangements in Ingenol Esters. *Australian Journal of Chemistry*, **2018**, 71, 212	1.2	4
34	Thermochemistry of Guanine Tautomers Re-Examined by Means of High-Level CCSD(T) Composite Ab Initio Methods. *Australian Journal of Chemistry*, **2019**, 72, 607	1.2	4
33	Thermochemical stabilities of giant fullerenes using density functional tight binding theory and isodesmic-type reactions. *Journal of Computational Chemistry*, **2021**, 42, 222-230	3.5	4
32	CCSDT(Q)/CBS thermochemistry for the D5h -kD10h isomerization in the C10 carbon cluster: Getting the right answer for the right reason. *Chemical Physics Letters*, **2018**, 706, 19-23	2.5	4
31	Empowering hydrogen storage properties of haeckelite monolayers via metal atom functionalization. *Applied Surface Science*, **2021**, 556, 149709	6.7	4
30	Investigation of an Unusual Crystal Habit of Hydrochlorothiazide Reveals Large Polar Enantiopure Domains and a Possible Crystal Nucleation Mechanism. *Angewandte Chemie*, **2019**, 131, 10361-10365	3.6	3
29	Thermochemistry of phosphorus sulfide cages: an extreme challenge for high-level ab initio methods. *Structural Chemistry*, **2019**, 30, 1665-1675	1.8	3
28	Benchmark study of DFT and composite methods for bond dissociation energies in argon compounds. *Chemical Physics*, **2020**, 531, 110676	2.3	3
27	Improved Adsorption and Migration of Divalent Ions Over C4N Nanosheets: Potential Anode for Divalent Batteries. *Surfaces and Interfaces*, **2020**, 21, 100758	4.1	3
26	Catalysis in Carbon Flatland-Flipping [8]Annulene on Graphene. *Chemistry - A European Journal*, **2021**, 27, 3420-3426	4.8	3
25	Prototypical dimers re-examined by means of high-level CCSDT(Q) composite ab initio methods. *Journal of Chemical Physics*, **2021**, 154, 124117	3.9	3
24	Perylene Bisimide Cyclophanes as Biaryl Enantiomerization Catalysts-Explorations into Catalysis and Host-Guest Chirality Transfer.. *Journal of Organic Chemistry*, **2022**,	4.2	2
23	Correlation between the energetic and thermal properties of C40 fullerene isomers: An accurate machine-learning force field study. *Micro and Nano Engineering*, **2022**, 14, 100105	3.4	2
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