

# Amir Karton

## List of Publications by Year in Descending Order

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**Version:** 2024-04-09

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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.

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	Perylene Bisimide Cyclophanes as Biaryl Enantiomerization Catalysts-Explorations into H-Catalysis and Host-Guest Chirality Transfer.. <i>Journal of Organic Chemistry</i> , <b>2022</b> ,	4.2	2
178	Superior performance of the machine-learning GAP force field for fullerene structures. <i>Structural Chemistry</i> , <b>2022</b> , 33, 505	1.8	1
177	Correlation between the energetic and thermal properties of C40 fullerene isomers: An accurate machine-learning force field study. <i>Micro and Nano Engineering</i> , <b>2022</b> , 14, 100105	3.4	2
176	Graphene-induced planarization of cyclooctatetraene derivatives. <i>Journal of Computational Chemistry</i> , <b>2022</b> , 43, 96-105	3.5	1
175	Extensive Redox Non-Innocence in Iron Bipyridine-Diimine Complexes: a Combined Spectroscopic and Computational Study. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 18296-18306	5.1	1
174	Comparative Study of Carbon Force Fields for the Simulation of Carbon Onions. <i>Australian Journal of Chemistry</i> , <b>2021</b> ,	1.2	2
173	High-level thermochemistry for the octasulfur ring: A converged coupled cluster perspective for a challenging second-row system. <i>Chemical Physics Impact</i> , <b>2021</b> , 3, 100047	1.6	2
172	Mechanistic insights into the autocatalyzed rearrangement of 2-bromooxazolines to 2-bromoisocyanates by means of high-level quantum chemical methods. <i>Journal of Physical Organic Chemistry</i> , <b>2021</b> , 34, e4214	2.1	
171	Evaluation of density functional theory for a large and diverse set of organic and inorganic equilibrium structures. <i>Journal of Computational Chemistry</i> , <b>2021</b> , 42, 1590-1601	3.5	14
170	Novel green phosphorene as a superior chemical gas sensing material. <i>Journal of Hazardous Materials</i> , <b>2021</b> , 401, 123340	12.8	32
169	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
168	Manganese-Catalyzed Hydroboration of Terminal Olefins and Metal-Dependent Selectivity in Internal Olefin Isomerization-Hydroboration. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 494-504	5.1	9
167	H-Catalysis in Carbon Flatland-Flipping [8]Annulene on Graphene. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 3420-3426	4.8	3
166	Scavenging properties of yttrium nitride monolayer towards toxic sulfur gases. <i>Applied Surface Science</i> , <b>2021</b> , 537, 147711	6.7	1
165	Can density functional theory cope with highly fluxional shapeshifting molecules?. <i>Chemical Physics</i> , <b>2021</b> , 540, 111013	2.3	5
164	Perylene bisimide cyclophanes as receptors for planar transition structures Catalysis of stereoinversions by shape-complementarity and noncovalent interactions. <i>Organic Chemistry Frontiers</i> , <b>2021</b> , 8, 4408-4418	5.2	2
163	Fluxionality by quantum tunnelling: nonclassical 21-homododecahedryl cation rearrangement re-revisited. <i>Chemical Communications</i> , <b>2021</b> , 57, 10735-10738	5.8	

162	Prototypical dimers re-examined by means of high-level CCSDT(Q) composite ab initio methods. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 124117	3.9	3
161	Accurate Heats of Formation for Polycyclic Aromatic Hydrocarbons: A High-Level Ab Initio Perspective. <i>Journal of Chemical &amp; Engineering Data</i> , <b>2021</b> , 66, 3453-3462	2.8	2
160	Empowering hydrogen storage properties of haeckelite monolayers via metal atom functionalization. <i>Applied Surface Science</i> , <b>2021</b> , 556, 149709	6.7	4
159	Can force fields developed for carbon nanomaterials describe the isomerization energies of fullerenes?. <i>Chemical Physics Letters</i> , <b>2021</b> , 779, 138853	2.5	6
158	Shapeshifting radicals. <i>Chemical Physics</i> , <b>2021</b> , 552, 111373	2.3	
157	Quantum mechanical tunnelling: the missing term to achieve sub-kJ mol barrier heights. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 10888-10898	3.6	6
156	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
155	Reactive Compression Molding Post-Inverse Vulcanization: A Method to Assemble, Recycle, and Repurpose Sulfur Polymers and Composites. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 10035-10044	4.8	29
154	Potassium Poly(Heptazine Imide): Transition Metal-Free Solid-State Triplet Sensitizer in Cascade Energy Transfer and [3+2]-cycloadditions. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 15061-15068	16.4	46
153	Chemically induced repair, adhesion, and recycling of polymers made by inverse vulcanization. <i>Chemical Science</i> , <b>2020</b> , 11, 5537-5546	9.4	37
152	Kalium-Polyheptazinimid: Ein Übergangsmetallfreier Festkörper-Triplett-Sensibilisator in Kaskadenenergietransfer und [3+2]-Cycloadditionen. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 15172-15180	3.6	9
151	Pristine Graphene as a Racemization Catalyst for Axially Chiral BINOL. <i>ChemPhysChem</i> , <b>2020</b> , 21, 1675-1681	9.8	7
150	Sensing of volatile organic compounds on two-dimensional nitrogenated holey graphene, graphdiyne, and their heterostructure. <i>Carbon</i> , <b>2020</b> , 163, 213-223	10.4	38
149	Criegee intermediate decomposition pathways for the formation of o-toluic acid and 2-methylphenylformate. <i>Chemical Physics Letters</i> , <b>2020</b> , 748, 137399	2.5	
148	The adsorption and migration behavior of divalent metals (Mg, Ca, and Zn) on pristine and defective graphene. <i>Carbon</i> , <b>2020</b> , 163, 276-287	10.4	17
147	Functionalized Two-Dimensional Nanoporous Graphene as Efficient Global Anode Materials for Li-, Na-, K-, Mg-, and Ca-Ion Batteries. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 9734-9745	3.8	17
146	Moiré patterns arising from bilayer graphone/graphene superlattice. <i>Nano Research</i> , <b>2020</b> , 13, 1060-1064	10	5
145	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

144	Remarkable improvement in hydrogen storage capacities of two-dimensional carbon nitride (g-C <sub>3</sub> N <sub>4</sub> ) nanosheets under selected transition metal doping. <i>International Journal of Hydrogen Energy</i> , <b>2020</b> , 45, 3035-3045	6.7	43
143	Theoretical Studies of SiCH Isomers Delineate Three Low-Lying Silylidenes Are Missing in the Laboratory. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 987-1002	2.8	13
142	Kinetics and Thermodynamics of Reactions Involving Criegee Intermediates: An Assessment of Density Functional Theory and Ab Initio Methods Through Comparison with CCSDT(Q)/CBS Data. <i>Journal of Computational Chemistry</i> , <b>2020</b> , 41, 328-339	3.5	10
141	Improved Adsorption and Migration of Divalent Ions Over C <sub>4</sub> N Nanosheets: Potential Anode for Divalent Batteries. <i>Surfaces and Interfaces</i> , <b>2020</b> , 21, 100758	4.1	3
140	Cope rearrangements in shapeshifting molecules re-examined by means of high-level CCSDT(Q) composite ab initio methods. <i>Chemical Physics Letters</i> , <b>2020</b> , 759, 138018	2.5	2
139	Effective basis set extrapolations for CCSDT, CCSDT(Q), and CCSDTQ correlation energies. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 024102	3.9	6
138	Catalysis on Pristine 2D Materials via Dispersion and Electrostatic Interactions. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 6977-6985	2.8	6
137	Atomistic simulations of the aggregation of small aromatic molecules in homogenous and heterogenous mixtures. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 21005-21014	3.6	2
136	Elemental Substitution of Two-Dimensional Transition Metal Dichalcogenides (MoSe and MoTe): Implications for Enhanced Gas Sensing. <i>ACS Sensors</i> , <b>2019</b> , 4, 2646-2653	9.2	42
135	Deciphering the exceptional selectivity of semipinacol rearrangements in cis-fused lactam diols using high-level quantum chemical methods. <i>Organic Chemistry Frontiers</i> , <b>2019</b> , 6, 725-731	5.2	5
134	Heterologous biosynthesis of elsinochrome A sheds light on the formation of the photosensitive perylenequinone system. <i>Chemical Science</i> , <b>2019</b> , 10, 1457-1465	9.4	44
133	Carnosine and Carcinine Derivatives Rapidly React with Hypochlorous Acid to Form Chloramines and Dichloramines. <i>Chemical Research in Toxicology</i> , <b>2019</b> , 32, 513-525	4	6
132	Toward Improved Performance of All-Organic Nitroxide Radical Batteries with Ionic Liquids: A Theoretical Perspective. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2019</b> , 7, 5367-5375	8.3	14
131	Thermoresponsive Graphene Membranes with Reversible Gating Regularity for Smart Fluid Control. <i>Advanced Functional Materials</i> , <b>2019</b> , 29, 1808501	15.6	43
130	Investigation of an Unusual Crystal Habit of Hydrochlorothiazide Reveals Large Polar Enantiopure Domains and a Possible Crystal Nucleation Mechanism. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 10361-10365	3.6	3
129	Investigation of an Unusual Crystal Habit of Hydrochlorothiazide Reveals Large Polar Enantiopure Domains and a Possible Crystal Nucleation Mechanism. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 10255-10259	16.4	6
128	Thermochemistry of phosphorus sulfide cages: an extreme challenge for high-level ab initio methods. <i>Structural Chemistry</i> , <b>2019</b> , 30, 1665-1675	1.8	3
127	Experimental and Theoretical Study of the Chemical Network of the Hydrogenation of NO on Interstellar Dust Grains. <i>ACS Earth and Space Chemistry</i> , <b>2019</b> , 3, 1196-1207	3.2	4

126	Reversible hydrogen storage properties of defect-engineered C4N nanosheets under ambient conditions. <i>Carbon</i> , <b>2019</b> , 152, 344-353	10.4	37
125	Blue phosphorene monolayers as potential nano sensors for volatile organic compounds under point defects. <i>Applied Surface Science</i> , <b>2019</b> , 486, 52-57	6.7	68
124	Enhancement in hydrogen storage capacities of light metal functionalized Boron Graphdiyne nanosheets. <i>Carbon</i> , <b>2019</b> , 147, 199-205	10.4	59
123	Spontaneous shape and phase control of colloidal ZnSe nanocrystals by tailoring Se precursor reactivity. <i>CrystEngComm</i> , <b>2019</b> , 21, 2955-2961	3.3	5
122	Thermochemistry of Guanine Tautomers Re-Examined by Means of High-Level CCSD(T) Composite Ab Initio Methods. <i>Australian Journal of Chemistry</i> , <b>2019</b> , 72, 607	1.2	4
121	Sensitivity enhancement of stanene towards toxic SO <sub>2</sub> and H <sub>2</sub> S. <i>Applied Surface Science</i> , <b>2019</b> , 495, 1436-1442	6.7	10
120	Catalysis by Pure Graphene-From Supporting Actor to Protagonist through Shape Complementarity. <i>Journal of Organic Chemistry</i> , <b>2019</b> , 84, 11343-11347	4.2	10
119	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. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 6720-6732	2.8	18
118	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
117	Theoretical Studies of Two Key Low-Lying Carbenes of CH Missing in the Laboratory. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 6618-6627	2.8	10
116	Basis set convergence of high-order coupled cluster methods up to CCSDTQ567 for a highly multireference molecule. <i>Chemical Physics Letters</i> , <b>2019</b> , 737, 136810	2.5	11
115	Macromolecular approach for targeted radioimmunotherapy in non-Hodgkin's lymphoma. <i>Chemical Communications</i> , <b>2019</b> , 55, 14506-14509	5.8	1
114	Efficient and selective sensing of nitrogen-containing gases by Si <sub>2</sub> BN nanosheets under pristine and pre-oxidized conditions. <i>Applied Surface Science</i> , <b>2019</b> , 469, 775-780	6.7	47
113	A computational foray into the mechanism and catalysis of the adduct formation reaction of guanine with crotonaldehyde. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 630-637	3.5	2
112	Performance of DFT for C Isomerization Energies: A Noticeable Exception to Jacob's Ladder. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 257-266	2.8	13
111	Metal functionalized inorganic nano-sheets as promising materials for clean energy storage. <i>Applied Surface Science</i> , <b>2019</b> , 471, 887-892	6.7	23
110	Tailoring the capability of carbon nitride (CN) nanosheets toward hydrogen storage upon light transition metal decoration. <i>Nanotechnology</i> , <b>2019</b> , 30, 075404	3.4	23
109	Accurate Thermochemical and Kinetic Stabilities of C Isomers. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 4768-4777	2.8	7

108	Dy <sub>3</sub> Al <sub>2</sub> (AlO <sub>4</sub> ) <sub>3</sub> ceramic nanogarnets: Sol-gel auto-combustion synthesis, characterization and joint experimental and computational structural analysis for electrochemical hydrogen storage performances. <i>Journal of Alloys and Compounds</i> , <b>2018</b> , 744, 574-582	5.7	26
107	A computational investigation of the sulphuric acid-catalysed 1,4-hydrogen transfer in higher Criegee intermediates. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25599	2.1	6
106	Predicting the primary fragments in mass spectrometry using ab initio Roby-Could bond indices. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25603	2.1	9
105	The High Performance of Choline Arginate for Biomass Pretreatment Is Due to Remarkably Strong Hydrogen Bonding by the Anion. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2018</b> , 6, 4115-4121	8.3	13
104	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. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 262, 204-217	6	26
103	Structure-Activity Studies of Semiochemicals from the Spider Orchid <i>Caladenia plicata</i> for Sexual Deception. <i>Journal of Chemical Ecology</i> , <b>2018</b> , 44, 436-443	2.7	7
102	Quantum chemical electron impact mass spectrum prediction for de novo structure elucidation: Assessment against experimental reference data and comparison to competitive fragmentation modeling. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25460	2.1	8
101	Post-CCSD(T) contributions to total atomization energies in multireference systems. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 034102	3.9	14
100	Mechanistic insights into the water-catalysed ring-opening reaction of vitamin E by means of double-hybrid density functional theory. <i>Chemical Physics Letters</i> , <b>2018</b> , 708, 123-129	2.5	1
99	Can Popular DFT Approximations and Truncated Coupled Cluster Theory Describe the Potential Energy Surface of the Beryllium Dimer?. <i>Australian Journal of Chemistry</i> , <b>2018</b> , 71, 804	1.2	5
98	Graphitic carbon nitride nano sheets functionalized with selected transition metal dopants: an efficient way to store CO. <i>Nanotechnology</i> , <b>2018</b> , 29, 415502	3.4	23
97	Covalency and Ionicity Do Not Oppose Each Other-Relationship Between Si-O Bond Character and Basicity of Siloxanes. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 15275-15286	4.8	28
96	A Computational Investigation of the Uncatalysed and Water-Catalysed Acyl Rearrangements in Ingenol Esters. <i>Australian Journal of Chemistry</i> , <b>2018</b> , 71, 212	1.2	4
95	The S66 Non-Covalent Interactions Benchmark Reconsidered Using Explicitly Correlated Methods Near the Basis Set Limit. <i>Australian Journal of Chemistry</i> , <b>2018</b> , 71, 238	1.2	30
94	Drastic Improvement in Gas-Sensing Characteristics of Phosphorene Nanosheets under Vacancy Defects and Elemental Functionalization. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 20186-20193	3.8	41
93	MVO-10: A Gas-Phase Oxide Benchmark for Localization/Delocalization in Mixed-Valence Systems. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 3512-3523	6.4	12
92	From High-Energy CH Isomers with A Planar Tetracoordinate Carbon Atom to An Experimentally Known Carbene. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 9054-9064	2.8	23
91	Bond orders for intermolecular interactions in crystals: charge transfer, ionicity and the effect on intramolecular bonds. <i>IUCrJ</i> , <b>2018</b> , 5, 635-646	4.7	16

90	The quest for the carbene bent-pentadiynylidene isomer of C <sub>5</sub> H <sub>2</sub> . <i>Chemical Physics</i> , <b>2018</b> , 515, 411-417	2.3	8
89	CCSDT(Q)/CBS thermochemistry for the D <sub>5h</sub> -D <sub>10h</sub> isomerization in the C <sub>10</sub> carbon cluster: Getting the right answer for the right reason. <i>Chemical Physics Letters</i> , <b>2018</b> , 706, 19-23	2.5	4
88	Proton enhanced dynamic battery chemistry for aprotic lithium-oxygen batteries. <i>Nature Communications</i> , <b>2017</b> , 8, 14308	17.4	88
87	Sulphuric acid-catalysed formation of hemiacetal from glyoxal and ethanol. <i>Chemical Physics Letters</i> , <b>2017</b> , 675, 27-34	2.5	5
86	An extended N-H bond, driven by a conserved second-order interaction, orients the flavin N5 orbital in cholesterol oxidase. <i>Scientific Reports</i> , <b>2017</b> , 7, 40517	4.9	9
85	Can DFT and ab initio methods adequately describe binding energies in strongly interacting C <sub>6</sub> X <sub>6</sub> ?C <sub>2</sub> X <sub>n</sub> complexes?. <i>Chemical Physics</i> , <b>2017</b> , 493, 12-19	2.3	1
84	Computational design of bio-inspired carnosine-based HOBr antioxidants. <i>Journal of Computer-Aided Molecular Design</i> , <b>2017</b> , 31, 905-913	4.2	5
83	W4-17: A diverse and high-confidence dataset of atomization energies for benchmarking high-level electronic structure methods. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 2063-2075	3.5	85
82	Sol-Gel auto-combustion synthesis and physicochemical properties of BaAl <sub>2</sub> O <sub>4</sub> nanoparticles; electrochemical hydrogen storage performance and density functional theory. <i>Renewable Energy</i> , <b>2017</b> , 114, 1419-1426	8.1	37
81	Computational insights for the hydride transfer and distinctive roles of key residues in cholesterol oxidase. <i>Scientific Reports</i> , <b>2017</b> , 7, 17265	4.9	9
80	Bioinspired graphene membrane with temperature tunable channels for water gating and molecular separation. <i>Nature Communications</i> , <b>2017</b> , 8, 2011	17.4	130
79	Energetic and spectroscopic properties of the low-lying CH isomers: a high-level ab initio perspective. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 17685-17697	3.6	13
78	How reliable is DFT in predicting relative energies of polycyclic aromatic hydrocarbon isomers? comparison of functionals from different rungs of Jacob's ladder. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 370-382	3.5	23
77	Stability of the chlorinated derivatives of the DNA/RNA nucleobases, purine and pyrimidine toward radical formation via homolytic C-Cl bond dissociation. <i>International Journal of Quantum Chemistry</i> , <b>2017</b> , 117, e25319	2.1	5
76	[Al <sub>2</sub> O <sub>4</sub> ] <sup>(-)</sup> , a Benchmark Gas-Phase Class II Mixed-Valence Radical Anion for the Evaluation of Quantum-Chemical Methods. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 3796-806	6.4	15
75	Restricted-Open-Shell G4(MP2)-Type Procedures. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 9299-9304	2.8	11
74	Geometries, interaction energies and complexation free energies of 18-crown-6 with neutral molecules. <i>CrystEngComm</i> , <b>2016</b> , 18, 8653-8663	3.3	1
73	Evaluation of the performance of MP4-based procedures for a wide range of thermochemical and kinetic properties. <i>Chemical Physics</i> , <b>2016</b> , 480, 23-35	2.3	8

72	Parapheromones for Thynnine Wasps. <i>Journal of Chemical Ecology</i> , <b>2016</b> , 42, 17-23	2.7	11
71	Heats of formation of platonic hydrocarbon cages by means of high-level thermochemical procedures. <i>Journal of Computational Chemistry</i> , <b>2016</b> , 37, 49-58	3.5	47
70	How large are post-CCSD(T) contributions to the total atomization energies of medium-sized alkanes?. <i>Chemical Physics Letters</i> , <b>2016</b> , 645, 118-122	2.5	12
69	Hydrogen Abstraction by OH and BH 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
68	Benchmark ab Initio Conformational Energies for the Proteinogenic Amino Acids through Explicitly Correlated Methods. Assessment of Density Functional Methods. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 444-54	6.4	75
67	Heat of formation for C <sub>60</sub> by means of the G4(MP2) thermochemical protocol through reactions in which C <sub>60</sub> is broken down into corannulene and sumanene. <i>Chemical Physics Letters</i> , <b>2016</b> , 643, 34-38	2.5	14
66	Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. <i>Molecular Physics</i> , <b>2016</b> , 114, 21-33	1.7	18
65	To bridge or not to bridge: The role of sulfuric acid in the Beckmann rearrangement. <i>Chemical Physics Letters</i> , <b>2016</b> , 659, 100-104	2.5	5
64	A computational chemist's guide to accurate thermochemistry for organic molecules. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2016</b> , 6, 292-310	7.9	137
63	Basis set convergence of CCSD(T) equilibrium geometries using a large and diverse set of molecular structures. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 104101	3.9	38
62	Toward a W4-F12 approach: Can explicitly correlated and orbital-based ab initio CCSD(T) limits be reconciled?. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 214101	3.9	69
61	A dataset of highly accurate homolytic N-Br bond dissociation energies obtained by Means of W2 theory. <i>International Journal of Quantum Chemistry</i> , <b>2016</b> , 116, 52-60	2.1	22
60	Mechanistic Insights into Water-Catalyzed Formation of Levoglucosenone from Anhydrosugar Intermediates by Means of High-Level Theoretical Procedures. <i>Australian Journal of Chemistry</i> , <b>2016</b> , 69, 943	1.2	13
59	Computational investigation into the gas-phase ozonolysis of the conjugated monoterpene $\beta$ -phellandrene. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 27991-28002	3.6	11
58	Thermochemistry of icosahedral closo-dicarbaboranes: a composite ab initio quantum-chemical perspective. <i>Canadian Journal of Chemistry</i> , <b>2016</b> , 94, 1082-1089	0.9	1
57	Reaction barrier heights for cycloreversion of heterocyclic rings: An Achilles'heel for DFT and standard ab initio procedures. <i>Chemical Physics</i> , <b>2015</b> , 458, 1-8	2.3	51
56	The CH <sub>3</sub> CHOO Criegee intermediate and its anion: Isomers, infrared spectra, and W3-F12 energetics. <i>Chemical Physics Letters</i> , <b>2015</b> , 621, 193-198	2.5	5
55	An assessment of theoretical procedures for $\pi$ -conjugation stabilisation energies in enones. <i>Molecular Physics</i> , <b>2015</b> , 113, 1284-1296	1.7	16

54	Estimating the CCSD basis-set limit energy from small basis sets: basis-set extrapolations vs additivity schemes. <i>AIP Advances</i> , <b>2015</b> , 5, 057148	1.5	10
53	Accurate reaction barrier heights of pericyclic reactions: Surprisingly large deviations for the CBS-QB3 composite method and their consequences in DFT benchmark studies. <i>Journal of Computational Chemistry</i> , <b>2015</b> , 36, 622-32	3.5	92
52	Pinning the most stable HxCyOz isomers in space by means of high-level theoretical procedures. <i>Chemical Physics</i> , <b>2014</b> , 436-437, 22-28	2.3	32
51	Inversion and rotation processes involving non-planar aromatic compounds catalyzed by extended polycyclic aromatic hydrocarbons. <i>Chemical Physics Letters</i> , <b>2014</b> , 614, 156-161	2.5	15
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45	A simple DFT-based diagnostic for nondynamical correlation. <i>Highlights in Theoretical Chemistry</i> , <b>2014</b> , 251-259		
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43	Evaluation of the heats of formation of corannulene and C <sub>60</sub> by means of high-level theoretical procedures. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 1834-42	2.8	42
42	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> , <b>2013</b> , 15, 7028-31	3.6	57
41	The melatonin conformer space: benchmark and assessment of wave function and DFT methods for a paradigmatic biological and pharmacological molecule. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 2269-77	2.8	77
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36	Assessment of theoretical procedures for calculating barrier heights for a diverse set of water-catalyzed proton-transfer reactions. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 4211-21	2.8	65
35	Heats of Formation for CrO, CrO <sub>2</sub> , and CrO <sub>3</sub> : 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
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33	Explicitly correlated Wn theory: W1-F12 and W2-F12. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 124114	3.9	176
32	Explicitly correlated benchmark calculations on C <sub>8</sub> H <sub>8</sub> isomer energy separations: how accurate are DFT, double-hybrid, and composite ab initio procedures?. <i>Molecular Physics</i> , <b>2012</b> , 110, 2477-2491	1.7	47
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30	Comment on "Revised electron affinity of SF <sub>6</sub> from kinetic data" [J. Chem. Phys. 136, 121102 (2012)]. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 197101	3.9	12
29	Model for the exceptional reactivity of peroxiredoxins 2 and 3 with hydrogen peroxide: a kinetic and computational study. <i>Journal of Biological Chemistry</i> , <b>2011</b> , 286, 18048-55	5.4	92
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27	Effect of substituents on the strength of N-X (X = H, F, and Cl) bond dissociation energies: a high-level quantum chemical study. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 5496-504	2.8	26
26	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. <i>Chemical Physics Letters</i> , <b>2011</b> , 510, 165-178	2.5	285
25	Performance of W4 theory for spectroscopic constants and electrical properties of small molecules. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 144102	3.9	56
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23	Post-CCSD(T) ab initio thermochemistry of halogen oxides and related hydrides XO <sub>x</sub> , XO <sub>2</sub> , HO <sub>x</sub> , XO <sub>n</sub> , and HXO <sub>n</sub> (X = F, Cl), and evaluation of DFT methods for these systems. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 4802-16	2.8	71
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