

# Mihaly Kallay

## List of Publications by Citations

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142  
papers

7,399  
citations

39  
h-index

84  
g-index

146  
ext. papers

8,098  
ext. citations

4  
avg, IF

6.34  
L-index

#	Paper	IF	Citations
142	Higher excitations in coupled-cluster theory. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 2945-2954	3.9	610
141	HEAT: High accuracy extrapolated ab initio thermochemistry. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 11599-613	3.9	606
140	W3 theory: robust computational thermochemistry in the kJ/mol accuracy range. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 4129-41	3.9	401
139	An efficient linear-scaling CCSD(T) method based on local natural orbitals. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 094105	3.9	294
138	Approximate treatment of higher excitations in coupled-cluster theory. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 214105	3.9	293
137	Coupled-cluster methods including noniterative corrections for quadruple excitations. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 054101	3.9	293
136	Calculation of excited-state properties using general coupled-cluster and configuration-interaction models. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 9257-69	3.9	288
135	High-accuracy extrapolated ab initio thermochemistry. II. Minor improvements to the protocol and a vital simplification. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 64108	3.9	277
134	A general state-selective multireference coupled-cluster algorithm. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 980-990	3.9	227
133	Basis-set extrapolation techniques for the accurate calculation of molecular equilibrium geometries using coupled-cluster theory. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 44108	3.9	203
132	Analytic calculation of the diagonal Born-Oppenheimer correction within configuration-interaction and coupled-cluster theory. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 144111	3.9	164
131	A general-order local coupled-cluster method based on the cluster-in-molecule approach. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 104111	3.9	160
130	State-of-the-art density matrix renormalization group and coupled cluster theory studies of the nitrogen binding curve. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 6110-6	3.9	155
129	Molecular equilibrium geometries based on coupled-cluster calculations including quadruple excitations. <i>Molecular Physics</i> , <b>2005</b> , 103, 2109-2115	1.7	155
128	Analytic second derivatives for general coupled-cluster and configuration-interaction models. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 6841-8	3.9	150
127	Analytic first derivatives for general coupled-cluster and configuration interaction models. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 2991-3004	3.9	138
126	The MRCC program system: Accurate quantum chemistry from water to proteins. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 074107	3.9	125

125	The barrier height of the F+H <sub>2</sub> reaction revisited: coupled-cluster and multireference configuration-interaction benchmark calculations. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 034305	3.9	122
124	Computing coupled-cluster wave functions with arbitrary excitations. <i>Journal of Chemical Physics</i> , <b>2000</b> , 113, 1359-1365	3.9	120
123	Full implementation and benchmark studies of Mukherjee's state-specific multireference coupled-cluster ansatz. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 074103	3.9	107
122	Approximate treatment of higher excitations in coupled-cluster theory. II. Extension to general single-determinant reference functions and improved approaches for the canonical Hartree-Fock case. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 144101	3.9	106
121	High-accuracy thermochemistry of atmospherically important fluorinated and chlorinated methane derivatives. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 13093-103	2.8	79
120	Linear-scaling implementation of the direct random-phase approximation. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 204105	3.9	74
119	Optimization of the Linear-Scaling Local Natural Orbital CCSD(T) Method: Improved Algorithm and Benchmark Applications. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 4193-4215	6.4	63
118	A non-fluorinated monobenzocyclooctyne for rapid copper-free click reactions. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 822-8	4.8	62
117	Exact density functional and wave function embedding schemes based on orbital localization. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 064107	3.9	59
116	Approaching the Basis Set Limit of CCSD(T) Energies for Large Molecules with Local Natural Orbital Coupled-Cluster Methods. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 5275-5298	6.4	58
115	High excitations in coupled-cluster series: vibrational energy levels of ammonia. <i>Molecular Physics</i> , <b>2004</b> , 102, 2297-2310	1.7	54
114	An Integral-Direct Linear-Scaling Second-Order Møller-Plesset Approach. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 4897-4914	6.4	53
113	Optimization of the linear-scaling local natural orbital CCSD(T) method: Redundancy-free triples correction using Laplace transform. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 214106	3.9	51
112	Calculation of electronic g-tensors using coupled cluster theory. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 11541-9	2.8	50
111	Construction and application of a new dual-hybrid random phase approximation. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 4615-26	6.4	48
110	Gauge-origin independent calculation of magnetizabilities and rotational g tensors at the coupled-cluster level. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 074101	3.9	46
109	A new family of bioorthogonally applicable fluorogenic labels. <i>Organic and Biomolecular Chemistry</i> , <b>2013</b> , 11, 3297-306	3.9	42
108	The origin of systematic error in the standard enthalpies of formation of hydrocarbons computed via atomization schemes. <i>ChemPhysChem</i> , <b>2006</b> , 7, 1664-7	3.2	42

107	Benchmark Thermochemistry of the Hydroperoxyl Radical $\square$ <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 3195-3199	2.8	41
106	Towards highly accurate ab initio thermochemistry of larger systems: benzene. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 044513	3.9	40
105	General implementation of the relativistic coupled-cluster method. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 234109	3.9	39
104	Equation-of-motion coupled-cluster methods for ionized states with an approximate treatment of triple excitations. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 154107	3.9	39
103	A systematic way for the cost reduction of density fitting methods. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 244113	3.9	36
102	Equilibrium Geometry of the Ethynyl (CCH) Radical $\square$ <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 3030-3034	2.8	36
101	Interactions, structure and properties in PLA/plasticized starch blends. <i>Polymer</i> , <b>2016</b> , 103, 9-18	3.9	35
100	On the protonation of water. <i>Chemical Science</i> , <b>2014</b> , 5, 3057-3063	9.4	35
99	Metal complexes of the merocyanine form of nitrobenzospyrans: Structure, optical spectra, stability. <i>Journal of Molecular Structure</i> , <b>2011</b> , 1000, 77-84	3.4	35
98	Relativistic general-order coupled-cluster method for high-precision calculations: Application to the Al <sup>+</sup> atomic clock. <i>Physical Review A</i> , <b>2011</b> , 83,	2.6	34
97	Calculation of frequency-dependent polarizabilities using general coupled-cluster models. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 768, 71-77		34
96	Reduced-cost linear-response CC2 method based on natural orbitals and natural auxiliary functions. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 194102	3.9	33
95	Electron Density Errors and Density-Driven Exchange-Correlation Energy Errors in Approximate Density Functional Calculations. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 4753-4764	6.4	33
94	High-accuracy theoretical thermochemistry of atmospherically important sulfur-containing molecules. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 7823-33	2.8	32
93	New generation of bioorthogonally applicable fluorogenic dyes with visible excitations and large Stokes shifts. <i>Bioconjugate Chemistry</i> , <b>2014</b> , 25, 1370-4	6.3	31
92	Inclusion of selected higher excitations involving active orbitals in the state-specific multireference coupled-cluster theory. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 234110	3.9	30
91	Integral-Direct and Parallel Implementation of the CCSD(T) Method: Algorithmic Developments and Large-Scale Applications. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 366-384	6.4	28
90	The accuracy of molecular bond lengths computed by multireference electronic structure methods. <i>Chemical Physics</i> , <b>2008</b> , 349, 37-57	2.3	27

89	Triplet State Characteristics of Higher Fullerenes. <i>Journal of Physical Chemistry A</i> , <b>1998</b> , 102, 1261-1273	2.8	26
88	Reduced-cost second-order algebraic-diagrammatic construction method for excitation energies and transition moments. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 094111	3.9	25
87	Superior performance of Mukherjee's state-specific multi-reference coupled-cluster theory at the singles and doubles truncation scheme with localized active orbitals. <i>Chemical Physics</i> , <b>2012</b> , 392, 83-89	2.3	25
86	Cost reduction of high-order coupled-cluster methods via active-space and orbital transformation techniques. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 124111	3.9	25
85	Calculation of frequency-dependent hyperpolarizabilities using general coupled-cluster models. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 134109	3.9	24
84	Construction of a Spin-Component Scaled Dual-Hybrid Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 796-803	6.4	23
83	Simple Modifications of the SCAN Meta-Generalized Gradient Approximation Functional. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 2469-2479	6.4	23
82	Chiral cyclohexane based fluorescent chemosensors for enantiomeric discrimination of aspartate. <i>Tetrahedron</i> , <b>2008</b> , 64, 3217-3224	2.4	23
81	Conditionally Activatable Visible-Light Photocages. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 15164-15171	16.4	23
80	Dual Basis Set Approach for Density Functional and Wave Function Embedding Schemes. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 4600-4615	6.4	22
79	Dissociation of the fluorine molecule. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 5518-28	2.8	22
78	Electronic structure of the singly bonded (C60) <sub>x</sub> fullerene polymer. <i>Physical Review B</i> , <b>1998</b> , 58, 3490-3493	3.3	22
77	Interactions between large molecules pose a puzzle for reference quantum mechanical methods. <i>Nature Communications</i> , <b>2021</b> , 12, 3927	17.4	22
76	Quantitative estimation of the strength of specific interactions in polyurethane elastomers, and their effect on structure and properties. <i>European Polymer Journal</i> , <b>2012</b> , 48, 1854-1865	5.2	21
75	High-accuracy theoretical thermochemistry of fluoroethanes. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 4824-36	2.8	20
74	Cinchona based squaramide catalysed enantioselective Michael addition of $\beta$ -nitro phosphonates to aryl acrylates: enantioselective synthesis of quaternary $\beta$ -aminophosphonates. <i>Tetrahedron: Asymmetry</i> , <b>2013</b> , 24, 1605-1614		19
73	High-accuracy theoretical study on the thermochemistry of several formaldehyde derivatives. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 13213-21	2.8	19
72	A Double-Clicking Bis-Azide Fluorogenic Dye for Bioorthogonal Self-Labeling Peptide Tags. <i>Chemistry - A European Journal</i> , <b>2016</b> , 22, 6382-8	4.8	19

71	A Simple Range-Separated Double-Hybrid Density Functional Theory for Excited States. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 927-942	6.4	19
70	Moderate-Cost Ab Initio Thermochemistry with Chemical Accuracy. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 4193-4204	6.4	18
69	Accurate Diels-Alder reaction energies from efficient density functional calculations. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 2879-88	6.4	17
68	Methylene blue $\alpha$ lixarenesulfonate supramolecular complexes and aggregates in aqueous solutions. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , <b>2009</b> , 207, 167-172	4.7	17
67	High-accuracy theoretical thermochemistry of atmospherically important nitrogen oxide derivatives. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 3144-53	2.8	16
66	On the role of high excitations in the intermolecular potential of H <sub>2</sub> O. <i>Molecular Physics</i> , <b>2006</b> , 104, 2337-2345	1.7	16
65	Femtosecond studies of charge-transfer mediated proton transfer in 2-butylamino-6-methyl-4-nitropyridine N-oxide. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 7086-91	2.8	16
64	High Accuracy Quantum Chemical and Thermochemical Network Data for the Heats of Formation of Fluorinated and Chlorinated Methanes and Ethanes. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 5993-6006	2.8	16
63	Experimental evidence of TICT state in 4-piperidinyl-1,8-naphthalimide - a kinetic and mechanistic study. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 10155-10164	3.6	15
62	The Cotton-Mouton effect of neon and argon: a benchmark study using highly correlated coupled cluster wave functions. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 9461-73	3.9	15
61	Crown ether derived from d-glucose as an efficient phase-transfer catalyst for the enantioselective Michael addition of malonates to enones. <i>Tetrahedron: Asymmetry</i> , <b>2016</b> , 27, 960-972		15
60	Thermochemical properties of small open-shell systems: experimental and high-level ab initio results for NH <sub>2</sub> and. <i>Molecular Physics</i> , <b>2006</b> , 104, 1457-1461	1.7	14
59	Asymmetric cyclopropanation reactions catalyzed by carbohydrate-based crown ethers. <i>Tetrahedron</i> , <b>2018</b> , 74, 3512-3526	2.4	13
58	Resolution of 1-n-propoxy-3-methyl-3-phospholene 1-oxide by diastereomeric complex formation using TADDOL derivatives and calcium salts of O,O'-dibenzoyl-(2R,3R)- or O,O'-di-p-toluoyl-(2R,3R)-tartaric acid. <i>Tetrahedron: Asymmetry</i> , <b>2014</b> , 25, 318-326		13
57	Analytic evaluation of Raman intensities in coupled-cluster theory. <i>Molecular Physics</i> , <b>2007</b> , 105, 2447-2453	4.3	13
56	Efficient singlet-state deactivation of cyano-substituted indolines in protic solvents via CN $\cdots$ HO hydrogen bonds. <i>ChemPhysChem</i> , <b>2007</b> , 8, 2627-35	3.2	13
55	On the convergence of the coupled-cluster sequence: the H8 model. <i>Computational and Theoretical Chemistry</i> , <b>2001</b> , 547, 145-151		13
54	Improving CISD calculations by geminal-type reference states. <i>Chemical Physics Letters</i> , <b>1999</b> , 312, 221-228		13

53	Synthesis and Evaluation of Nicotinic Acid Derived Tetrazines for Bioorthogonal Labeling. <i>Synthesis</i> , <b>2015</b> , 47, 2738-2744	2.9	12
52	Supramolecular FRET modulation by pseudorotaxane formation of a ditopic stilbazolium dye and carboxylato-pillar[5]arene. <i>Dyes and Pigments</i> , <b>2016</b> , 133, 415-423	4.6	12
51	Resolution of 1-n-butyl-3-methyl-3-phospholene 1-oxide with TADDOL derivatives and calcium salts of O,O'-Dibenzoyl-(2R,3R)- or O,O'-di-p-toluoyl-(2R,3R)-tartaric acid. <i>Chirality</i> , <b>2014</b> , 26, 174-82	2.1	12
50	Solvation and protonation of coumarin 102 in aqueous media: a fluorescence spectroscopic and theoretical study. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 5238-47	2.8	12
49	Nonconventional partitioning of the many-body Hamiltonian for studying correlation effects. <i>International Journal of Quantum Chemistry</i> , <b>1998</b> , 70, 571-581	2.1	12
48	Adsorption of an active molecule on the surface of halloysite for controlled release application: Interaction, orientation, consequences. <i>Applied Clay Science</i> , <b>2016</b> , 132-133, 167-174	5.2	12
47	The kinetics and mechanism of photooxygenation of 4'-diethylamino-3-hydroxyflavone. <i>Photochemical and Photobiological Sciences</i> , <b>2016</b> , 15, 219-27	4.2	11
46	On the Miller condition in the equation-of-motion method: ionization potentials from multi-reference wave functions. <i>Physical Chemistry Chemical Physics</i> , <b>2001</b> , 3, 696-701	3.6	11
45	Accurate Reduced-Cost CCSD(T) Energies: Parallel Implementation, Benchmarks, and Large-Scale Applications. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 860-878	6.4	11
44	A study on the optical resolution of 1-isopropyl-3-methyl-3-phospholene 1-oxide and its use in the synthesis of borane and platinum complexes. <i>Journal of Organometallic Chemistry</i> , <b>2015</b> , 797, 140-152	2.3	10
43	A Case Study on the Resolution of the 1-i-Butyl-3-methyl-3-phospholene 1-Oxide via Diastereomeric Complex Formation Using TADDOL Derivatives and via Diastereomeric Coordination Complexes Formed from the Calcium Salts of O,O'-Diaroyl-(2R,3R)-tartaric Acids. <i>Heteroatom Chemistry</i> , <b>2015</b> , 26, 79-90	1.2	10
42	Efficient evaluation of three-center Coulomb integrals. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 204101	3.9	9
41	Reduced-Scaling Correlation Methods for the Excited States of Large Molecules: Implementation and Benchmarks for the Second-Order Algebraic-Diagrammatic Construction Approach. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 6111-6126	6.4	9
40	Theoretical study on the photooxygenation and photorearrangement reactions of 3-hydroxyflavone. <i>RSC Advances</i> , <b>2017</b> , 7, 32185-32192	3.7	9
39	A quasiparticle-based multi-reference coupled-cluster method. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 134112	3.9	9
38	Assignment of absolute configurations of chiral phospholene oxides by UV/CD spectroscopy using TD-DFT quantum chemical calculations and singular value decomposition approach for the analysis of the spectra. <i>Computational and Theoretical Chemistry</i> , <b>2009</b> , 906, 94-99		9
37	Spin-Scaled Range-Separated Double-Hybrid Density Functional Theory for Excited States. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 4211-4224	6.4	9
36	Synthesis, Characterization, and Application of Platinum(II) Complexes Incorporating Racemic and Optically Active 4-Chloro-5-Methyl-1-Phenyl-1,2,3,6-Tetrahydrophosphinine Ligand. <i>Heteroatom Chemistry</i> , <b>2016</b> , 27, 91-101	1.2	9

35	Combined Density Functional and Algebraic-Diagrammatic Construction Approach for Accurate Excitation Energies and Transition Moments. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 4440-4453 <sup>8</sup>	6.4	8
34	Theoretical and thermochemical network approaches to determine the heats of formation for HO <sub>2</sub> and its ionic counterparts. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 1164-76	2.8	8
33	Unconventional bond functions for quantum chemical calculations. <i>Theoretical Chemistry Accounts</i> , <b>2015</b> , 134, 1	1.9	7
32	An uracil-linked hydroxyflavone probe for the recognition of ATP. <i>Beilstein Journal of Organic Chemistry</i> , <b>2018</b> , 14, 747-755	2.5	7
31	Construction of a Range-Separated Dual-Hybrid Direct Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 6678-6687	6.4	7
30	Energetics and zero-field-splitting in triplet states of C70. <i>Computational and Theoretical Chemistry</i> , <b>1997</b> , 398-399, 293-300		7
29	Enthalpy Differences of the n-Pentane Conformers. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 2679-88	6.4	7
28	Accurate Theoretical Thermochemistry for Fluoroethyl Radicals. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 1153-1162	2.8	6
27	Reduced-Scaling Approach for Configuration Interaction Singles and Time-Dependent Density Functional Theory Calculations Using Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 1690-1704	6.4	6
26	Synthesis of a poly(2-azanorbornene) with a high degree of cis-TT-stereoregularity and a regular secondary solution structure. <i>Polymer Chemistry</i> , <b>2012</b> , 3, 2760	4.9	6
25	Benchmark theoretical study on the dissociation energy of chlorine. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 7765-72	2.8	6
24	Hydrogen bonding effects on the fluorescence properties of 4'-diethylamino-3-hydroxyflavone in water and water-acetone mixtures. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2018</b> , 203, 96-105	4.4	6
23	Reducing the Many-Electron Self-Interaction Error in the Second-Order Screened Exchange Method. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 6607-6616	6.4	5
22	A QM/MM program using frozen localized orbitals and the Huzinaga equation. <i>Theoretical Chemistry Accounts</i> , <b>2015</b> , 134, 1	1.9	5
21	Oxygen reduction reaction on TiO <sub>2</sub> rutile (1 1 0) surface in the presence of bridging hydroxyl groups. <i>Computational and Theoretical Chemistry</i> , <b>2019</b> , 1168, 112607	2	5
20	The $\pi$ -Electron Delocalization in 2-Oxazolines Revisited: Quantification and Comparison with Its Analogue in Esters. <i>Materials</i> , <b>2015</b> , 8, 5385-5397	3.5	5
19	Linear-Scaling Open-Shell MP2 Approach: Algorithm, Benchmarks, and Large-Scale Applications. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 2886-2905	6.4	5
18	Size-consistent explicitly correlated triple excitation correction. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 034107	3.9	5



17	Circular dichroism spectra of trans-chalcone epoxides. <i>Tetrahedron: Asymmetry</i> , <b>2007</b> , 18, 1521-1528		4
16	Speeding up Hartree-Fock and Kohn-Sham calculations with first-order corrections. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 164114	3.9	3
15	Synthesis and characterization of isophorondiamine-based oligoamides: catalytic effect of amides during the curing of epoxy resins. <i>Polymer Bulletin</i> , <b>2020</b> , 77, 4655-4678	2.4	3
14	Strong ion pair charge transfer interaction of 1,8-naphthalimideBipyridinium conjugates with basic anions Towards the development of a new type of turn-on fluorescent anion sensors. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 6666-6674	3.6	2
13	Binding Modes of a Phenylpyridinium Styryl Fluorescent Dye with Cucurbiturils. <i>Molecules</i> , <b>2020</b> , 25,	4.8	2
12	Speeding up density fitting HartreeFock calculations with multipole approximations. <i>Molecular Physics</i> , <b>2020</b> , 118, e1769213	1.7	2
11	Novel strategy to implement active-space coupled-cluster methods. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 124108	3.9	2
10	Triplet State Characteristics of Smaller Fullerenes. <i>Fullerenes, Nanotubes, and Carbon Nanostructures</i> , <b>1997</b> , 5, 355-373		2
9	Accurate Spectral Properties within Double-Hybrid Density Functional Theory: A Spin-Scaled Range-Separated Second-Order Algebraic-Diagrammatic Construction-Based Approach.. <i>Journal of Chemical Theory and Computation</i> , <b>2022</b> ,	6.4	2
8	Oxygen Reduction Reaction on N-Doped Graphene: Effect of Positions and Scaling Relations of Adsorption Energies. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 8551-8561	3.8	2
7	Basis set truncation corrections for improved frozen natural orbital CCSD(T) energies. <i>Molecular Physics</i> , e1963495	1.7	2
6	Thermochemistry of Uracil, Thymine, Cytosine, and Adenine. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 4057-4067	2.8	1
5	A second-order multi-reference quasiparticle-based perturbation theory. <i>Theoretical Chemistry Accounts</i> , <b>2015</b> , 134, 1	1.9	1
4	Multilevel approach to the initial guess for self-consistent field calculations. <i>International Journal of Quantum Chemistry</i> , e26782	2.1	1
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1	Preface to the special collection of theoretical chemistry accounts in honour of PĀer R. SurjĀ. <i>Theoretical Chemistry Accounts</i> , <b>2016</b> , 135, 1	1.9	