Mihaly Kallay

List of Publications by Year
in descending order

145 papers	8,859 citations	61984 43 h-index	43889 91 g-index
146 all docs	146 docs citations	146 times ranked	4380 citing authors

#	Article	IF	Citations
1	HEAT: High accuracy extrapolatedab initiothermochemistry. Journal of Chemical Physics, 2004, 121, 11599-11613.	3.0	691
2	Higher excitations in coupled-cluster theory. Journal of Chemical Physics, 2001, 115, 2945-2954.	3.0	666
3	W3 theory: Robust computational thermochemistry in the kJ/mol accuracy range. Journal of Chemical Physics, 2004, 120, 4129-4141.	3.0	434
4	Coupled-cluster methods including noniterative corrections for quadruple excitations. Journal of Chemical Physics, 2005, 123, 054101.	3.0	344
5	Approximate treatment of higher excitations in coupled-cluster theory. Journal of Chemical Physics, 2005, 123, 214105.	3.0	344
6	An efficient linear-scaling CCSD(T) method based on local natural orbitals. Journal of Chemical Physics, 2013, 139, 094105.	3.0	324
7	Calculation of excited-state properties using general coupled-cluster and configuration-interaction models. Journal of Chemical Physics, 2004, 121, 9257-9269.	3.0	319
8	High-accuracy extrapolated ab initio thermochemistry. II. Minor improvements to the protocol and a vital simplification. Journal of Chemical Physics, 2006, 125, 064108.	3.0	312
9	The MRCC program system: Accurate quantum chemistry from water to proteins. Journal of Chemical Physics, 2020, 152, 074107.	3.0	264
10	A general state-selective multireference coupled-cluster algorithm. Journal of Chemical Physics, 2002, 117, 980-990.	3.0	237
11	Basis-set extrapolation techniques for the accurate calculation of molecular equilibrium geometries using coupled-cluster theory. Journal of Chemical Physics, 2006, 125, 044108.	3.0	233
12	Analytic calculation of the diagonal Born-Oppenheimer correction within configuration-interaction and coupled-cluster theory. Journal of Chemical Physics, 2006, 125, 144111.	3.0	182
13	A general-order local coupled-cluster method based on the cluster-in-molecule approach. Journal of Chemical Physics, 2011, 135, 104111.	3.0	181
14	Molecular equilibrium geometries based on coupled-cluster calculations including quadruple excitations. Molecular Physics, 2005, 103, 2109-2115.	1.7	176
15	State-of-the-art density matrix renormalization group and coupled cluster theory studies of the nitrogen binding curve. Journal of Chemical Physics, 2004, 121, 6110-6116.	3.0	172
16	Analytic second derivatives for general coupled-cluster and configuration-interaction models. Journal of Chemical Physics, 2004, 120, 6841-6848.	3.0	163
17	Analytic first derivatives for general coupled-cluster and configuration interaction models. Journal of Chemical Physics, 2003, 119, 2991-3004.	3.0	152
18	The barrier height of the F+H2 reaction revisited: Coupled-cluster and multireference configuration-interaction benchmark calculations. Journal of Chemical Physics, 2008, 128, 034305.	3.0	136

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19	Approximate treatment of higher excitations in coupled-cluster theory. II. Extension to general single-determinant reference functions and improved approaches for the canonical Hartreeâ€“Fock case. Journal of Chemical Physics, 2008, 129, 144101.	3.0	128
20	Computing coupled-cluster wave functions with arbitrary excitations. Journal of Chemical Physics, 2000, 113, 1359-1365.	3.0	127
21	Full implementation and benchmark studies of Mukherjeeâ€™s state-specific multireference coupled-cluster ansatz. Journal of Chemical Physics, 2010, 132, 074103.	3.0	114
22	Approaching the Basis Set Limit of CCSD(T) Energies for Large Molecules with Local Natural Orbital Coupled-Cluster Methods. Journal of Chemical Theory and Computation, 2019, 15, 5275-5298.	5.3	112
23	Optimization of the Linear-Scaling Local Natural Orbital CCSD(T) Method: Improved Algorithm and Benchmark Applications. Journal of Chemical Theory and Computation, 2018, 14, 4193-4215.	5.3	94
24	Linear-scaling implementation of the direct random-phase approximation. Journal of Chemical Physics, 2015, 142, 204105.	3.0	92
25	High-Accuracy Thermochemistry of Atmospherically Important Fluorinated and Chlorinated Methane Derivatives. Journal of Physical Chemistry A, 2010, 114, 13093-13103.	2.5	85
26	Exact density functional and wave function embedding schemes based on orbital localization. Journal of Chemical Physics, 2016, 145, .	3.0	80
27	An Integral-Direct Linear-Scaling Second-Order MÃ¸llerâ€“Plesset Approach. Journal of Chemical Theory and Computation, 2016, 12, 4897-4914.	5.3	72
28	Optimization of the linear-scaling local natural orbital CCSD(T) method: Redundancy-free triples correction using Laplace transform. Journal of Chemical Physics, 2017, 146, 214106.	3.0	70
29	A Nonâ€Fluorinated Monobenzocyclooctyne for Rapid Copperâ€Free Click Reactions. Chemistry - A European Journal, 2012, 18, 822-828.	3.3	65
30	Calculation of Electronicg-Tensors using Coupled Cluster Theory. Journal of Physical Chemistry A, 2009, 113, 11541-11549.	2.5	58
31	High excitations in coupled-cluster series: vibrational energy levels of ammonia. Molecular Physics, 2004, 102, 2297-2310.	1.7	57
32	Interactions between large molecules pose a puzzle for reference quantum mechanical methods. Nature Communications, 2021, 12, 3927.	12.8	57
33	Conditionally Activatable Visible-Light Photocages. Journal of the American Chemical Society, 2020, 142, 15164-15171.	13.7	56
34	Construction and Application of a New Dual-Hybrid Random Phase Approximation. Journal of Chemical Theory and Computation, 2015, 11, 4615-4626.	5.3	54
35	Gauge-origin independent calculation of magnetizabilities and rotational g tensors at the coupled-cluster level. Journal of Chemical Physics, 2007, 127, 074101.	3.0	53
36	Interactions, structure and properties in PLA/plasticized starch blends. Polymer, 2016, 103, 9-18.	3.8	50

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37	General implementation of the relativistic coupled-cluster method. Journal of Chemical Physics, 2010, 133, 234109.	3.0	48
38	A systematic way for the cost reduction of density fitting methods. Journal of Chemical Physics, 2014, 141, 244113.	3.0	48
39	Electron Density Errors and Density-Driven Exchange-Correlation Energy Errors in Approximate Density Functional Calculations. Journal of Chemical Theory and Computation, 2017, 13, 4753-4764.	5.3	48
40	Reduced-cost linear-response CC2 method based on natural orbitals and natural auxiliary functions. Journal of Chemical Physics, 2017, 146, 194102.	3.0	47
41	A new family of bioorthogonally applicable fluorogenic labels. Organic and Biomolecular Chemistry, 2013, 11, 3297.	2.8	46
42	Integral-Direct and Parallel Implementation of the CCSD(T) Method: Algorithmic Developments and Large-Scale Applications. Journal of Chemical Theory and Computation, 2020, 16, 366-384.	5.3	46
43	The Origin of Systematic Error in the Standard Enthalpies of Formation of Hydrocarbons Computed via Atomization Schemes. ChemPhysChem, 2006, 7, 1664-1667.	2.1	45
44	Equation-of-motion coupled-cluster methods for ionized states with an approximate treatment of triple excitations. Journal of Chemical Physics, 2005, 122, 154107.	3.0	44
45	Towards highly accurate ab initio thermochemistry of larger systems: Benzene. Journal of Chemical Physics, 2011, 135, 044513.	3.0	44
46	Benchmark Thermochemistry of the Hydroperoxyl Radicalâ€. Journal of Physical Chemistry A, 2004, 108, 3195-3199.	2.5	43
47	Relativistic general-order coupled-cluster method for high-precision calculations: Application to the Al<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:mrow></mml:math>atomic clock. Physical Review A, 2011, 83, .	2.5	41
48	On the protonation of water. Chemical Science, 2014, 5, 3057-3063.	7.4	41
49	Equilibrium Geometry of the Ethynyl (CCH) Radicalâ€. Journal of Physical Chemistry A, 2004, 108, 3030-3034.	2.5	39
50	Metal complexes of the merocyanine form of nitrobenzospyran: Structure, optical spectra, stability. Journal of Molecular Structure, 2011, 1000, 77-84.	3.6	38
51	A Simple Range-Separated Double-Hybrid Density Functional Theory for Excited States. Journal of Chemical Theory and Computation, 2021, 17, 927-942.	5.3	38
52	Reduced-cost second-order algebraic-diagrammatic construction method for excitation energies and transition moments. Journal of Chemical Physics, 2018, 148, .	3.0	37
53	Calculation of frequency-dependent polarizabilities using general coupled-cluster models. Computational and Theoretical Chemistry, 2006, 768, 71-77.	1.5	36
54	High-Accuracy Theoretical Thermochemistry of Atmospherically Important Sulfur-Containing Molecules. Journal of Physical Chemistry A, 2011, 115, 7823-7833.	2.5	36

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55	New Generation of Bioorthogonally Applicable Fluorogenic Dyes with Visible Excitations and Large Stokes Shifts. Bioconjugate Chemistry, 2014, 25, 1370-1374.	3.6	34
56	Inclusion of selected higher excitations involving active orbitals in the state-specific multireference coupled-cluster theory. Journal of Chemical Physics, 2010, 133, 234110.	3.0	33
57	Accurate Reduced-Cost CCSD(T) Energies: Parallel Implementation, Benchmarks, and Large-Scale Applications. Journal of Chemical Theory and Computation, 2021, 17, 860-878.	5.3	32
58	Charge-Transfer Excitations within Density Functional Theory: How Accurate Are the Most Recommended Approaches?. Journal of Chemical Theory and Computation, 2022, 18, 1646-1662.	5.3	30
59	Dual Basis Set Approach for Density Functional and Wave Function Embedding Schemes. Journal of Chemical Theory and Computation, 2018, 14, 4600-4615.	5.3	29
60	Cost reduction of high-order coupled-cluster methods via active-space and orbital transformation techniques. Journal of Chemical Physics, 2011, 134, 124111.	3.0	28
61	Calculation of frequency-dependent hyperpolarizabilities using general coupled-cluster models. Journal of Chemical Physics, 2007, 127, 134109.	3.0	27
62	The accuracy of molecular bond lengths computed by multireference electronic structure methods. Chemical Physics, 2008, 349, 37-57.	1.9	27
63	Experimental evidence of TICT state in 4-piperidinyl-1,8-naphthalimide â€“ a kinetic and mechanistic study. Physical Chemistry Chemical Physics, 2018, 20, 10155-10164.	2.8	27
64	Triplet State Characteristics of Higher Fullerenes. Journal of Physical Chemistry A, 1998, 102, 1261-1273.	2.5	26
65	Superior performance of Mukherjeeâ€™s state-specific multi-reference coupled-cluster theory at the singles and doubles truncation scheme with localized active orbitals. Chemical Physics, 2012, 392, 83-89.	1.9	26
66	Simple Modifications of the SCAN Meta-Generalized Gradient Approximation Functional. Journal of Chemical Theory and Computation, 2018, 14, 2469-2479.	5.3	26
67	Chiral cyclohexane based fluorescent chemosensors for enantiomeric discrimination of aspartate. Tetrahedron, 2008, 64, 3217-3224.	1.9	25
68	Construction of a Spin-Component Scaled Dual-Hybrid Random Phase Approximation. Journal of Chemical Theory and Computation, 2017, 13, 796-803.	5.3	25
69	Spin-Scaled Range-Separated Double-Hybrid Density Functional Theory for Excited States. Journal of Chemical Theory and Computation, 2021, 17, 4211-4224.	5.3	25
70	High-Accuracy Theoretical Thermochemistry of Fluoroethanes. Journal of Physical Chemistry A, 2014, 118, 4824-4836.	2.5	24
71	A Doubleâ€Clicking Bisâ€Azide Fluorogenic Dye for Bioorthogonal Selfâ€Labeling Peptide Tags. Chemistry - A European Journal, 2016, 22, 6382-6388.	3.3	24
72	Quantitative estimation of the strength of specific interactions in polyurethane elastomers, and their effect on structure and properties. European Polymer Journal, 2012, 48, 1854-1865.	5.4	23

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73	Electronic structure of the singly bonded(C60)xfullerene polymer. Physical Review B, 1998, 58, 3490-3493.	3.2	22
74	Cinchona based squaramide catalysed enantioselective Michael addition of Î±-nitrophosphonates to aryl acrylates: enantioselective synthesis of quaternary Î±-aminophosphonates. Tetrahedron: Asymmetry, 2013, 24, 1605-1614.	1.8	22
75	Dissociation of the Fluorine Molecule. Journal of Physical Chemistry A, 2013, 117, 5518-5528.	2.5	22
76	Crown ether derived from d-glucose as an efficient phase-transfer catalyst for the enantioselective Michael addition of malonates to enones. Tetrahedron: Asymmetry, 2016, 27, 960-972.	1.8	22
77	Moderate-Cost Ab Initio Thermochemistry with Chemical Accuracy. Journal of Chemical Theory and Computation, 2017, 13, 4193-4204.	5.3	22
78	Asymmetric cyclopropanation reactions catalyzed by carbohydrate-based crown ethers. Tetrahedron, 2018, 74, 3512-3526.	1.9	21
79	Combined Density Functional and Algebraic-Diagrammatic Construction Approach for Accurate Excitation Energies and Transition Moments. Journal of Chemical Theory and Computation, 2019, 15, 4440-4453.	5.3	21
80	High Accuracy Quantum Chemical and Thermochemical Network Data for the Heats of Formation of Fluorinated and Chlorinated Methanes and Ethanes. Journal of Physical Chemistry A, 2018, 122, 5993-6006.	2.5	20
81	Femtosecond Studies of Charge-Transfer Mediated Proton Transfer in 2-Butylamino-6-methyl-4-nitropyridineN-Oxide. Journal of Physical Chemistry A, 2006, 110, 7086-7091.	2.5	19
82	High-Accuracy Theoretical Study on the Thermochemistry of Several Formaldehyde Derivatives. Journal of Physical Chemistry A, 2010, 114, 13213-13221.	2.5	19
83	Accurate Dielsâ€“Alder Reaction Energies from Efficient Density Functional Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2879-2888.	5.3	19
84	Oxygen Reduction Reaction on N-Doped Graphene: Effect of Positions and Scaling Relations of Adsorption Energies. Journal of Physical Chemistry C, 2021, 125, 8551-8561.	3.1	19
85	Size-consistent explicitly correlated triple excitation correction. Journal of Chemical Physics, 2021, 155, 034107.	3.0	19
86	High-Accuracy Theoretical Thermochemistry of Atmospherically Important Nitrogen Oxide Derivatives. Journal of Physical Chemistry A, 2011, 115, 3144-3153.	2.5	18
87	Reduced-Scaling Correlation Methods for the Excited States of Large Molecules: Implementation and Benchmarks for the Second-Order Algebraic-Diagrammatic Construction Approach. Journal of Chemical Theory and Computation, 2019, 15, 6111-6126.	5.3	18
88	Methylene blueâ€“calixarenesulfonate supramolecular complexes and aggregates in aqueous solutions. Journal of Photochemistry and Photobiology A: Chemistry, 2009, 207, 167-172.	3.9	17
89	Improving CISD calculations by geminal-type reference states. Chemical Physics Letters, 1999, 312, 221-228.	2.6	16
90	The Cotton-Mouton effect of neon and argon: A benchmark study using highly correlated coupled cluster wave functions. Journal of Chemical Physics, 2004, 121, 9461-9473.	3.0	16

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91	On the role of high excitations in the intermolecular potential of H2â€“CO. Molecular Physics, 2006, 104, 2337-2345.	1.7	16
92	Linear-Scaling Open-Shell MP2 Approach: Algorithm, Benchmarks, and Large-Scale Applications. Journal of Chemical Theory and Computation, 2021, 17, 2886-2905.	5.3	16
93	On the â€œkiller conditionâ€™' in the equation-of-motion method: ionization potentials from multi-reference wave functions. Physical Chemistry Chemical Physics, 2001, 3, 696-701.	2.8	15
94	On the convergence of the coupled-cluster sequence: the H8 model. Computational and Theoretical Chemistry, 2001, 547, 145-151.	1.5	15
95	Thermochemical properties of small open-shell systems: experimental and high-levelab initioresults for NH2and. Molecular Physics, 2006, 104, 1457-1461.	1.7	15
96	Solvation and Protonation of Coumarin 102 in Aqueous Media: A Fluorescence Spectroscopic and Theoretical Study. Journal of Physical Chemistry A, 2014, 118, 5238-5247.	2.5	15
97	Efficient Singletâ€State Deactivation of Cyanoâ€Substituted Indolines in Protic Solvents via CNï£¿HO Hydrogen Bonds. ChemPhysChem, 2007, 8, 2627-2635.	2.1	14
98	Resolution of 1â€nâ€Butylâ€3â€Methylâ€3â€Phospholene 1â€Oxide With TADDOL Derivatives and Calcium Salts of O,O'â€Dibenzoylâ€(2R,3R)â€or O,O'â€diâ€pâ€Toluoylâ€(2R,3R)â€tartaric Acid. Chirality, 2014, 26, 174-182.	2.6	14
99	Synthesis and Evaluation of Nicotinic Acid Derived Tetrazines for Bioorthogonal Labeling. Synthesis, 2015, 47, 2738-2744.	2.3	14
100	The kinetics and mechanism of photooxygenation of 4â€²-diethylamino-3-hydroxyflavone. Photochemical and Photobiological Sciences, 2016, 15, 219-227.	2.9	14
101	Accurate Spectral Properties within Double-Hybrid Density Functional Theory: A Spin-Scaled Range-Separated Second-Order Algebraic-Diagrammatic Construction-Based Approach. Journal of Chemical Theory and Computation, 2022, 18, 865-882.	5.3	14
102	Analytic evaluation of Raman intensities in coupled-cluster theory. Molecular Physics, 2007, 105, 2447-2453.	1.7	13
103	Resolution of 1-n-propoxy-3-methyl-3-phospholene 1-oxide by diastereomeric complex formation using TADDOL derivatives and calcium salts of O,Oâ€²-dibenzoyl-(2R,3R)- or O,Oâ€²-di-p-toluoyl-(2R,3R)-tartaric acid. Tetrahedron: Asymmetry, 2014, 25, 318-326.	1.8	13
104	Adsorption of an active molecule on the surface of halloysite for controlled release application: Interaction, orientation, consequences. Applied Clay Science, 2016, 132-133, 167-174.	5.2	13
105	Supramolecular FRET modulation by pseudorotaxane formation of a ditopic stilbazolium dye and carboxylato-pillar[5]arene. Dyes and Pigments, 2016, 133, 415-423.	3.7	13
106	Efficient evaluation of three-center Coulomb integrals. Journal of Chemical Physics, 2017, 146, 204101.	3.0	13
107	Nonconventional partitioning of the many-body Hamiltonian for studying correlation effects. International Journal of Quantum Chemistry, 1998, 70, 571-581.	2.0	12
108	Hydrogen bonding effects on the fluorescence properties of 4â€²-diethylamino-3-hydroxyflavone in water and water-acetone mixtures. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 96-105.	3.9	12

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109	A Case Study on the Resolution of the 1â€iâ€Butylâ€3â€methylâ€3â€phospholene 1â€Oxide via Diastereomeric Complex Formation Using TADDOL Derivatives and via Diastereomeric Coordination Complexes Formed from the Calcium Salts of O,Oâ€²â€Diaroylâ€(2R,3R)â€tartaric Acids. Heteroatom Chemistry, 2015, 26, 79-90.	0.7	11
110	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. Journal of Organometallic Chemistry, 2015, 797, 140-152.	1.8	11
111	Theoretical study on the photooxygenation and photorearrangement reactions of 3-hydroxyflavone. RSC Advances, 2017, 7, 32185-32192.	3.6	11
112	An uracil-linked hydroxyflavone probe for the recognition of ATP. Beilstein Journal of Organic Chemistry, 2018, 14, 747-755.	2.2	11
113	Oxygen reduction reaction on TiO2 rutile (1â€¯1â€¯0) surface in the presence of bridging hydroxyl groups. Computational and Theoretical Chemistry, 2019, 1168, 112607.	2.5	11
114	A quasiparticle-based multi-reference coupled-cluster method. Journal of Chemical Physics, 2014, 141, 134112.	3.0	10
115	Theoretical and Thermochemical Network Approaches To Determine the Heats of Formation for HO₂ and Its Ionic Counterparts. Journal of Physical Chemistry A, 2015, 119, 1164-1176.	2.5	10
116	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. Heteroatom Chemistry, 2016, 27, 91-101.	0.7	10
117	Construction of a Range-Separated Dual-Hybrid Direct Random Phase Approximation. Journal of Chemical Theory and Computation, 2019, 15, 6678-6687.	5.3	10
118	Reduced-Scaling Approach for Configuration Interaction Singles and Time-Dependent Density Functional Theory Calculations Using Hybrid Functionals. Journal of Chemical Theory and Computation, 2019, 15, 1690-1704.	5.3	10
119	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. Computational and Theoretical Chemistry, 2009, 906, 94-99.	1.5	9
120	Enthalpy Differences of then-Pentane Conformers. Journal of Chemical Theory and Computation, 2016, 12, 2679-2688.	5.3	9
121	A pillararene-based indicator displacement assay for the fluorescence detection of vitamin B1. Sensors and Actuators B: Chemical, 2022, 369, 132364.	7.8	9
122	Accurate Theoretical Thermochemistry for Fluoroethyl Radicals. Journal of Physical Chemistry A, 2017, 121, 1153-1162.	2.5	8
123	Reducing the Many-Electron Self-Interaction Error in the Second-Order Screened Exchange Method. Journal of Chemical Theory and Computation, 2019, 15, 6607-6616.	5.3	8
124	Energetics and zero-field-splitting in triplet states of C70. Computational and Theoretical Chemistry, 1997, 398-399, 293-300.	1.5	7
125	Synthesis of a poly(2-azanorbornene) with a high degree of cis-TT-stereoregularity and a regular secondary solution structure. Polymer Chemistry, 2012, 3, 2760.	3.9	7
126	The Ï€-Electron Delocalization in 2-Oxazolines Revisited: Quantification and Comparison with Its Analogue in Esters. Materials, 2015, 8, 5385-5397.	2.9	7

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127	Unconventional bond functions for quantum chemical calculations. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	7
128	Synthesis and characterization of isophorondiamine-based oligoamides: catalytic effect of amides during the curing of epoxy resins. Polymer Bulletin, 2020, 77, 4655-4678.	3.3	7
129	Basis set truncation corrections for improved frozen natural orbital CCSD(T) energies. Molecular Physics, 2021, 119, .	1.7	7
130	Benchmark Theoretical Study on the Dissociation Energy of Chlorine. Journal of Physical Chemistry A, 2011, 115, 7765-7772.	2.5	6
131	A QM/MM program using frozen localized orbitals and the Huzinaga equation. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	6
132	Thermochemistry of Uracil, Thymine, Cytosine, and Adenine. Journal of Physical Chemistry A, 2019, 123, 4057-4067.	2.5	6
133	Circular dichroism spectra of trans-chalcone epoxides. Tetrahedron: Asymmetry, 2007, 18, 1521-1528.	1.8	5
134	Strong ion pair charge transfer interaction of 1,8-naphthalimideâ€“bipyridinium conjugates with basic anions â€“ towards the development of a new type of turn-on fluorescent anion sensors. New Journal of Chemistry, 2019, 43, 6666-6674.	2.8	5
135	Binding Modes of a Phenylpyridinium Styryl Fluorescent Dye with Cucurbiturils. Molecules, 2020, 25, 5111.	3.8	5
136	Speeding up Hartreeâ€“Fock and Kohnâ€“Sham calculations with first-order corrections. Journal of Chemical Physics, 2021, 154, 164114.	3.0	5
137	Speeding up density fitting Hartreeâ€“Fock calculations with multipole approximations. Molecular Physics, 2020, 118, e1769213.	1.7	4
138	A second-order multi-reference quasiparticle-based perturbation theory. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	3
139	Multilevel approach to the initial guess for selfâ€consistent field calculations. International Journal of Quantum Chemistry, 2022, 122, e26782.	2.0	3
140	Triplet State Characteristics of Smaller Fullerenes. Fullerenes, Nanotubes, and Carbon Nanostructures, 1997, 5, 355-373.	0.6	2
141	Novel strategy to implement active-space coupled-cluster methods. Journal of Chemical Physics, 2018, 148, 124108.	3.0	2
142	Efficient evaluation of the geometrical first derivatives of three-center Coulomb integrals. Journal of Chemical Physics, 2018, 149, 124101.	3.0	2
143	Implementation and Optimization of the Embedded Cluster Reference Interaction Site Model with Atomic Charges. Journal of Physical Chemistry A, 2022, 126, 2417-2429.	2.5	1
144	Preface to the special collection of theoretical chemistry accounts in honour of PÃ©ter R. SurjÃ¡n. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	0

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145	Preparation of enantiopure 1â€isopentylâ€3â€methylâ€3â€phospholene 1â€oxide via the formation of diastereomeric complexes. Heteroatom Chemistry, 2018, 29, .	0.7	0