Mihaly Kallay

List of Publications by Year in Descending Order

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	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**,	6.4	2
141	Speeding up Hartree-Fock and Kohn-Sham calculations with first-order corrections. *Journal of Chemical Physics*, **2021**, 154, 164114	3.9	3
140	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	3.8	2
139	Linear-Scaling Open-Shell MP2 Approach: Algorithm, Benchmarks, and Large-Scale Applications. *Journal of Chemical Theory and Computation*, **2021**, 17, 2886-2905	6.4	5
138	Interactions between large molecules pose a puzzle for reference quantum mechanical methods. *Nature Communications*, **2021**, 12, 3927	17.4	22
137	Spin-Scaled Range-Separated Double-Hybrid Density Functional Theory for Excited States. *Journal of Chemical Theory and Computation*, **2021**, 17, 4211-4224	6.4	9
136	Size-consistent explicitly correlated triple excitation correction. *Journal of Chemical Physics*, **2021**, 155, 034107	3.9	5
135	Accurate Reduced-Cost CCSD(T) Energies: Parallel Implementation, Benchmarks, and Large-Scale Applications. *Journal of Chemical Theory and Computation*, **2021**, 17, 860-878	6.4	11
134	A Simple Range-Separated Double-Hybrid Density Functional Theory for Excited States. *Journal of Chemical Theory and Computation*, **2021**, 17, 927-942	6.4	19
133	Binding Modes of a Phenylpyridinium Styryl Fluorescent Dye with Cucurbiturils. *Molecules*, **2020**, 25,	4.8	2
132	Speeding up density fitting Hartree–Fock calculations with multipole approximations. *Molecular Physics*, **2020**, 118, e1769213	1.7	2
131	The MRCC program system: Accurate quantum chemistry from water to proteins. *Journal of Chemical Physics*, **2020**, 152, 074107	3.9	125
130	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	6.4	28
129	Conditionally Activatable Visible-Light Photocages. *Journal of the American Chemical Society*, **2020**, 142, 15164-15171	16.4	23
128	Synthesis and characterization of isophorondiamine-based oligoamides: catalytic effect of amides during the curing of epoxy resins. *Polymer Bulletin*, **2020**, 77, 4655-4678	2.4	3
127	Reducing the Many-Electron Self-Interaction Error in the Second-Order Screened Exchange Method. *Journal of Chemical Theory and Computation*, **2019**, 15, 6607-6616	6.4	5
126	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	6.4	58

125	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	6.4	9
124	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	6.4	6
123	Strong ion pair charge transfer interaction of 1,8-naphthalimide-bipyridinium conjugates with basic anions – towards the development of a new type of turn-on fluorescent anion sensors. *New Journal of Chemistry*, **2019**, 43, 6666-6674	3.6	2
122	Thermochemistry of Uracil, Thymine, Cytosine, and Adenine. *Journal of Physical Chemistry A*, **2019**, 123, 4057-4067	2.8	1
121	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	6.4	8
120	Oxygen reduction reaction on TiO2 rutile (1 1 0) surface in the presence of bridging hydroxyl groups. *Computational and Theoretical Chemistry*, **2019**, 1168, 112607	2	5
119	Construction of a Range-Separated Dual-Hybrid Direct Random Phase Approximation. *Journal of Chemical Theory and Computation*, **2019**, 15, 6678-6687	6.4	7
118	Reduced-cost second-order algebraic-diagrammatic construction method for excitation energies and transition moments. *Journal of Chemical Physics*, **2018**, 148, 094111	3.9	25
117	Preparation of enantiopure 1-isopentyl-3-methyl-3-phospholene 1-oxide via the formation of diastereomeric complexes. *Heteroatom Chemistry*, **2018**, 29, e21411	1.2	
116	Asymmetric cyclopropanation reactions catalyzed by carbohydrate-based crown ethers. *Tetrahedron*, **2018**, 74, 3512-3526	2.4	13
115	Simple Modifications of the SCAN Meta-Generalized Gradient Approximation Functional. *Journal of Chemical Theory and Computation*, **2018**, 14, 2469-2479	6.4	23
114	Experimental evidence of TICT state in 4-piperidinyl-1,8-naphthalimide - a kinetic and mechanistic study. *Physical Chemistry Chemical Physics*, **2018**, 20, 10155-10164	3.6	15
113	Novel strategy to implement active-space coupled-cluster methods. *Journal of Chemical Physics*, **2018**, 148, 124108	3.9	2
112	An uracil-linked hydroxyflavone probe for the recognition of ATP. *Beilstein Journal of Organic Chemistry*, **2018**, 14, 747-755	2.5	7
111	Dual Basis Set Approach for Density Functional and Wave Function Embedding Schemes. *Journal of Chemical Theory and Computation*, **2018**, 14, 4600-4615	6.4	22
110	Efficient evaluation of the geometrical first derivatives of three-center Coulomb integrals. *Journal of Chemical Physics*, **2018**, 149, 124101	3.9	1
109	Hydrogen bonding effects on the fluorescence properties of 4'-diethylamino-3-hydroxyflavone in water and water-acetone mixtures. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2018**, 203, 96-105	4.4	6
108	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	2.8	16

107	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	6.4	63
106	Accurate Theoretical Thermochemistry for Fluoroethyl Radicals. *Journal of Physical Chemistry A*, **2017**, 121, 1153-1162	2.8	6
105	Reduced-cost linear-response CC2 method based on natural orbitals and natural auxiliary functions. *Journal of Chemical Physics*, **2017**, 146, 194102	3.9	33
104	Efficient evaluation of three-center Coulomb integrals. *Journal of Chemical Physics*, **2017**, 146, 204101	3.9	9
103	Construction of a Spin-Component Scaled Dual-Hybrid Random Phase Approximation. *Journal of Chemical Theory and Computation*, **2017**, 13, 796-803	6.4	23
102	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	6.4	33
101	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	3.9	51
100	Moderate-Cost Ab Initio Thermochemistry with Chemical Accuracy. *Journal of Chemical Theory and Computation*, **2017**, 13, 4193-4204	6.4	18
99	Theoretical study on the photooxygenation and photorearrangement reactions of 3-hydroxyflavone. *RSC Advances*, **2017**, 7, 32185-32192	3.7	9
98	Interactions, structure and properties in PLA/plasticized starch blends. *Polymer*, **2016**, 103, 9-18	3.9	35
97	An Integral-Direct Linear-Scaling Second-Order M□ller-Plesset Approach. *Journal of Chemical Theory and Computation*, **2016**, 12, 4897-4914	6.4	53
96	Supramolecular FRET modulation by pseudorotaxane formation of a ditopic stilbazolium dye and carboxylato-pillar[5]arene. *Dyes and Pigments*, **2016**, 133, 415-423	4.6	12
95	The kinetics and mechanism of photooxygenation of 4'-diethylamino-3-hydroxyflavone. *Photochemical and Photobiological Sciences*, **2016**, 15, 219-27	4.2	11
94	Preface to the special collection of theoretical chemistry accounts in honour of P□er R. Surj□. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	
93	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	12
92	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	1.2	9
91	A Double-Clicking Bis-Azide Fluorogenic Dye for Bioorthogonal Self-Labeling Peptide Tags. *Chemistry - A European Journal*, **2016**, 22, 6382-8	4.8	19
90	Exact density functional and wave function embedding schemes based on orbital localization. *Journal of Chemical Physics*, **2016**, 145, 064107	3.9	59

89	Enthalpy Differences of the n-Pentane Conformers. *Journal of Chemical Theory and Computation*, **2016**, 12, 2679-88	6.4	7
88	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		15
87	Accurate Diels-Alder reaction energies from efficient density functional calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 2879-88	6.4	17
86	Unconventional bond functions for quantum chemical calculations. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	7
85	A QM/MM program using frozen localized orbitals and the Huzinaga equation. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	5
84	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	2.3	10
83	Synthesis and Evaluation of Nicotinic Acid Derived Tetrazines for Bioorthogonal Labeling. *Synthesis*, **2015**, 47, 2738-2744	2.9	12
82	Construction and application of a new dual-hybrid random phase approximation. *Journal of Chemical Theory and Computation*, **2015**, 11, 4615-26	6.4	48
81	The Electron Delocalization in 2-Oxazolines Revisited: Quantification and Comparison with Its Analogue in Esters. *Materials*, **2015**, 8, 5385-5397	3.5	5
80	Linear-scaling implementation of the direct random-phase approximation. *Journal of Chemical Physics*, **2015**, 142, 204105	3.9	74
79	A second-order multi-reference quasiparticle-based perturbation theory. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	1
78	Theoretical and thermochemical network approaches to determine the heats of formation for HO2 and its ionic counterparts. *Journal of Physical Chemistry A*, **2015**, 119, 1164-76	2.8	8
77	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 ofO,O?-Diaroyl-(2R,3R)-tartaric Acids. *Heteroatom Chemistry*, **2015**, 26, 79-90	1.2	10
76	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. *Tetrahedron: Asymmetry*, **2014**, 25, 318-326		13
75	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. *Chirality*, **2014**, 26, 174-82	2.1	12
74	High-accuracy theoretical thermochemistry of fluoroethanes. *Journal of Physical Chemistry A*, **2014**, 118, 4824-36	2.8	20
73	On the protonation of water. *Chemical Science*, **2014**, 5, 3057-3063	9.4	35
72	Solvation and protonation of coumarin 102 in aqueous media: a fluorescence spectroscopic and theoretical study. *Journal of Physical Chemistry A*, **2014**, 118, 5238-47	2.8	12

71	New generation of bioorthogonally applicable fluorogenic dyes with visible excitations and large Stokes shifts. *Bioconjugate Chemistry*, **2014**, 25, 1370-4	6.3	31
70	A systematic way for the cost reduction of density fitting methods. *Journal of Chemical Physics*, **2014**, 141, 244113	3.9	36
69	A quasiparticle-based multi-reference coupled-cluster method. *Journal of Chemical Physics*, **2014**, 141, 134112	3.9	9
68	Cinchona based squaramide catalysed enantioselective Michael addition of α-nitrophosphonates to aryl acrylates: enantioselective synthesis of quaternary α-aminophosphonates. *Tetrahedron: Asymmetry*, **2013**, 24, 1605-1614		19
67	An efficient linear-scaling CCSD(T) method based on local natural orbitals. *Journal of Chemical Physics*, **2013**, 139, 094105	3.9	294
66	A new family of bioorthogonally applicable fluorogenic labels. *Organic and Biomolecular Chemistry*, **2013**, 11, 3297-306	3.9	42
65	Dissociation of the fluorine molecule. *Journal of Physical Chemistry A*, **2013**, 117, 5518-28	2.8	22
64	A non-fluorinated monobenzocyclooctyne for rapid copper-free click reactions. *Chemistry - A European Journal*, **2012**, 18, 822-8	4.8	62
63	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	5.2	21
62	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	4.9	6
61	Superior performance of Mukherjee'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	2.3	25
60	Cost reduction of high-order coupled-cluster methods via active-space and orbital transformation techniques. *Journal of Chemical Physics*, **2011**, 134, 124111	3.9	25
59	High-accuracy theoretical thermochemistry of atmospherically important nitrogen oxide derivatives. *Journal of Physical Chemistry A*, **2011**, 115, 3144-53	2.8	16
58	A general-order local coupled-cluster method based on the cluster-in-molecule approach. *Journal of Chemical Physics*, **2011**, 135, 104111	3.9	160
57	Metal complexes of the merocyanine form of nitrobenzospyran: Structure, optical spectra, stability. *Journal of Molecular Structure*, **2011**, 1000, 77-84	3.4	35
56	High-accuracy theoretical thermochemistry of atmospherically important sulfur-containing molecules. *Journal of Physical Chemistry A*, **2011**, 115, 7823-33	2.8	32
55	Benchmark theoretical study on the dissociation energy of chlorine. *Journal of Physical Chemistry A*, **2011**, 115, 7765-72	2.8	6
54	Relativistic general-order coupled-cluster method for high-precision calculations: Application to the Al+ atomic clock. *Physical Review A*, **2011**, 83,	2.6	34

53	Towards highly accurate ab initio thermochemistry of larger systems: benzene. *Journal of Chemical Physics*, **2011**, 135, 044513	3.9	40
52	Inclusion of selected higher excitations involving active orbitals in the state-specific multireference coupled-cluster theory. *Journal of Chemical Physics*, **2010**, 133, 234110	3.9	30
51	High-accuracy theoretical study on the thermochemistry of several formaldehyde derivatives. *Journal of Physical Chemistry A*, **2010**, 114, 13213-21	2.8	19
50	High-accuracy thermochemistry of atmospherically important fluorinated and chlorinated methane derivatives. *Journal of Physical Chemistry A*, **2010**, 114, 13093-103	2.8	79
49	Full implementation and benchmark studies of Mukherjee's state-specific multireference coupled-cluster ansatz. *Journal of Chemical Physics*, **2010**, 132, 074103	3.9	107
48	General implementation of the relativistic coupled-cluster method. *Journal of Chemical Physics*, **2010**, 133, 234109	3.9	39
47	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		9
46	Methylene blue–calixarenesulfonate supramolecular complexes and aggregates in aqueous solutions. *Journal of Photochemistry and Photobiology A: Chemistry*, **2009**, 207, 167-172	4.7	17
45	Calculation of electronic g-tensors using coupled cluster theory. *Journal of Physical Chemistry A*, **2009**, 113, 11541-9	2.8	50
44	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. *Journal of Chemical Physics*, **2008**, 129, 144101	3.9	106
43	Chiral cyclohexane based fluorescent chemosensors for enantiomeric discrimination of aspartate. *Tetrahedron*, **2008**, 64, 3217-3224	2.4	23
42	The accuracy of molecular bond lengths computed by multireference electronic structure methods. *Chemical Physics*, **2008**, 349, 37-57	2.3	27
41	The barrier height of the F+H2 reaction revisited: coupled-cluster and multireference configuration-interaction benchmark calculations. *Journal of Chemical Physics*, **2008**, 128, 034305	3.9	122
40	Analytic evaluation of Raman intensities in coupled-cluster theory. *Molecular Physics*, **2007**, 105, 2447-2453	1.7	13
39	Efficient singlet-state deactivation of cyano-substituted indolines in protic solvents via CN--HO hydrogen bonds. *ChemPhysChem*, **2007**, 8, 2627-35	3.2	13
38	Circular dichroism spectra of trans-chalcone epoxides. *Tetrahedron: Asymmetry*, **2007**, 18, 1521-1528		4
37	Gauge-origin independent calculation of magnetizabilities and rotational g tensors at the coupled-cluster level. *Journal of Chemical Physics*, **2007**, 127, 074101	3.9	46
36	Calculation of frequency-dependent hyperpolarizabilities using general coupled-cluster models. *Journal of Chemical Physics*, **2007**, 127, 134109	3.9	24

35	The origin of systematic error in the standard enthalpies of formation of hydrocarbons computed via atomization schemes. *ChemPhysChem*, **2006**, 7, 1664-7	3.2	42
34	On the role of high excitations in the intermolecular potential of H2□O. *Molecular Physics*, **2006**, 104, 2337-2345	1.7	16
33	High-accuracy extrapolated ab initio thermochemistry. II. Minor improvements to the protocol and a vital simplification. *Journal of Chemical Physics*, **2006**, 125, 64108	3.9	277
32	Basis-set extrapolation techniques for the accurate calculation of molecular equilibrium geometries using coupled-cluster theory. *Journal of Chemical Physics*, **2006**, 125, 44108	3.9	203
31	Femtosecond studies of charge-transfer mediated proton transfer in 2-butylamino-6-methyl-4-nitropyridine N-oxide. *Journal of Physical Chemistry A*, **2006**, 110, 7086-91	2.8	16
30	Analytic calculation of the diagonal Born-Oppenheimer correction within configuration-interaction and coupled-cluster theory. *Journal of Chemical Physics*, **2006**, 125, 144111	3.9	164
29	Thermochemical properties of small open-shell systems: experimental and high-level ab initio results for NH2 and. *Molecular Physics*, **2006**, 104, 1457-1461	1.7	14
28	Calculation of frequency-dependent polarizabilities using general coupled-cluster models. *Computational and Theoretical Chemistry*, **2006**, 768, 71-77		34
27	Approximate treatment of higher excitations in coupled-cluster theory. *Journal of Chemical Physics*, **2005**, 123, 214105	3.9	293
26	Molecular equilibrium geometries based on coupled-cluster calculations including quadruple excitations. *Molecular Physics*, **2005**, 103, 2109-2115	1.7	155
25	Equation-of-motion coupled-cluster methods for ionized states with an approximate treatment of triple excitations. *Journal of Chemical Physics*, **2005**, 122, 154107	3.9	39
24	Coupled-cluster methods including noniterative corrections for quadruple excitations. *Journal of Chemical Physics*, **2005**, 123, 054101	3.9	293
23	HEAT: High accuracy extrapolated ab initio thermochemistry. *Journal of Chemical Physics*, **2004**, 121, 11599-613	3.9	606
22	W3 theory: robust computational thermochemistry in the kJ/mol accuracy range. *Journal of Chemical Physics*, **2004**, 120, 4129-41	3.9	401
21	Calculation of excited-state properties using general coupled-cluster and configuration-interaction models. *Journal of Chemical Physics*, **2004**, 121, 9257-69	3.9	288
20	The Cotton-Mouton effect of neon and argon: a benchmark study using highly correlated coupled cluster wave functions. *Journal of Chemical Physics*, **2004**, 121, 9461-73	3.9	15
19	Benchmark Thermochemistry of the Hydroperoxyl Radical□*Journal of Physical Chemistry A*, **2004**, 108, 3195-3199	2.8	41
18	Equilibrium Geometry of the Ethynyl (CCH) Radical□*Journal of Physical Chemistry A*, **2004**, 108, 3030-3034	2.8	36

17	High excitations in coupled-cluster series: vibrational energy levels of ammonia. *Molecular Physics*, **2004**, 102, 2297-2310	1.7	54
16	State-of-the-art density matrix renormalization group and coupled cluster theory studies of the nitrogen binding curve. *Journal of Chemical Physics*, **2004**, 121, 6110-6	3.9	155
15	Analytic second derivatives for general coupled-cluster and configuration-interaction models. *Journal of Chemical Physics*, **2004**, 120, 6841-8	3.9	150
14	Analytic first derivatives for general coupled-cluster and configuration interaction models. *Journal of Chemical Physics*, **2003**, 119, 2991-3004	3.9	138
13	A general state-selective multireference coupled-cluster algorithm. *Journal of Chemical Physics*, **2002**, 117, 980-990	3.9	227
12	On the convergence of the coupled-cluster sequence: the H8 model. *Computational and Theoretical Chemistry*, **2001**, 547, 145-151		13
11	Higher excitations in coupled-cluster theory. *Journal of Chemical Physics*, **2001**, 115, 2945-2954	3.9	610
10	On the killer condition in the equation-of-motion method: ionization potentials from multi-reference wave functions. *Physical Chemistry Chemical Physics*, **2001**, 3, 696-701	3.6	11
9	Computing coupled-cluster wave functions with arbitrary excitations. *Journal of Chemical Physics*, **2000**, 113, 1359-1365	3.9	120
8	Improving CISD calculations by geminal-type reference states. *Chemical Physics Letters*, **1999**, 312, 221-228	2.3	13
7	Nonconventional partitioning of the many-body Hamiltonian for studying correlation effects. *International Journal of Quantum Chemistry*, **1998**, 70, 571-581	2.1	12
6	Triplet State Characteristics of Higher Fullerenes. *Journal of Physical Chemistry A*, **1998**, 102, 1261-1273	2.8	26
5	Electronic structure of the singly bonded (C60)x fullerene polymer. *Physical Review B*, **1998**, 58, 3490-3493	3.3	22
4	Triplet State Characteristics of Smaller Fullerenes. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **1997**, 5, 355-373		2
3	Energetics and zero-field-splitting in triplet states of C70. *Computational and Theoretical Chemistry*, **1997**, 398-399, 293-300		7
2	Multilevel approach to the initial guess for self-consistent field calculations. *International Journal of Quantum Chemistry*,e26782	2.1	1
1	Basis set truncation corrections for improved frozen natural orbital CCSD(T) energies. *Molecular Physics*,e1963495	1.7	2