Ludwik Adamowicz

List of Publications by Year
in descending order

283	6,925	71102	91884
papers	citations	41 h-index	69 g-index

283	283	283	2740
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A stateâ€selective multireference coupledâ€cluster theory employing the singleâ€reference formalism. Journal of Chemical Physics, 1993, 99, 1875-1900.	3.0	300
2	Multireference coupledâ€cluster method using a singleâ€reference formalism. Journal of Chemical Physics, 1991, 94, 1229-1235.	3.0	282
3	Theory and application of explicitly correlated Gaussians. Reviews of Modern Physics, 2013, 85, 693-749.	45.6	263
4	Coupledâ€cluster method truncated at quadruples. Journal of Chemical Physics, 1991, 95, 6645-6651.	3.0	214
5	Stateâ€selective multireference coupledâ€cluster theory employing the singleâ€reference formalism: Implementation and application to the H8 model system. Journal of Chemical Physics, 1994, 100, 5792-5809.	3.0	192
6	The implementation of the multireference coupledâ€cluster method based on the singleâ€reference formalism. Journal of Chemical Physics, 1992, 96, 3739-3744.	3.0	156
7	Non-Bornâ€“Oppenheimer calculations of atoms and molecules. Physical Chemistry Chemical Physics, 2003, 5, 1491-1501.	2.8	141
8	Bornâ€“Oppenheimer and Non-Bornâ€“Oppenheimer, Atomic and Molecular Calculations with Explicitly Correlated Gaussians. Chemical Reviews, 2013, 113, 36-79.	47.7	129
9	The infrared spectra of matrix isolated uracil and thymine: An assignment based on new theoretical calculations. Spectrochimica Acta Part A: Molecular Spectroscopy, 1992, 48, 1385-1395.	0.1	117
10	Computing relative stabilities of metallofullerenes by Gibbs energy treatments. Theoretical Chemistry Accounts, 2007, 117, 315-322.	1.4	104
11	Improved computational strategy for the stateâ€selective coupledâ€cluster theory with semiâ€internal triexcited clusters: Potential energy surface of the HF molecule. Journal of Chemical Physics, 1995, 103, 9331-9346.	3.0	95
12	Improved Nonadiabatic Ground-State Energy Upper Bound for Dihydrogen. Physical Review Letters, 1999, 83, 2541-2543.	7.8	89
13	Dipole-Bound Electron Attachment to Uracilâ‹¯Water Complexes. Theoreticalab InitioStudy. The Journal of Physical Chemistry, 1996, 100, 14655-14660.	2.9	77
14	Multireference coupled cluster method for electronic structure of molecules. International Reviews in Physical Chemistry, 1993, 12, 339-362.	2.3	75
15	Search for Stable Anions of Uracilâ‹¯Water Clusters. Ab Initio Theoretical Studies. Journal of Physical Chemistry A, 1997, 101, 9152-9156.	2.5	75
16	CASCCD: Coupled-cluster method with double excitations and the CAS reference. Journal of Chemical Physics, 2000, 112, 9258-9268.	3.0	72
17	Five lowest<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mmultiscripts><mml:mi>S</mml:mi><mml:mprescripts /><mml:none /><mml:mn>1</mml:mn></mml:mmultiscripts></mml:mrow></mml:math>states of the Be atom calculated with a finite-nuclear-mass approach and with relativistic and QED corrections. Physical Review A, 2009, 80, .	2.5	72
18	Non-Born-Oppenheimer Variational Calculations of Atoms and Molecules with Explicitly Correlated Gaussian Basis Functions. Advances in Chemical Physics, 2005, , 377-475.	0.3	70

#	Article	IF	Citations
19	Breaking bonds with the stateâ€selective multireference coupledâ€cluster method employing the singleâ€reference formalism. Journal of Chemical Physics, 1995, 102, 898-904.	3.0	68
20	A correlated basis set for nonadiabatic energy calculations on diatomic molecules. Journal of Chemical Physics, 1999, 110, 7166-7175.	3.0	68
21	Molecular structure in non-Bornâ€“Oppenheimer quantum mechanics. Chemical Physics Letters, 2004, 387, 136-141.	2.6	65
22	An effective method for generating nonadiabatic manyâ€body wave function using explicitly correlated Gaussianâ€type functions. Journal of Chemical Physics, 1991, 95, 6681-6698.	3.0	61
23	Beryllium atom reinvestigated: A comparison between theory and experiment. Physical Review A, 1991, 43, 3355-3364.	2.5	59
24	Covalent Anion of the Canonical Adenineâ‹¯Thymine Base Pair. Ab Initio Study. Journal of Physical Chemistry A, 2000, 104, 2994-2998.	2.5	59
25	Ab initio theoretical study of dipole-bound anions of molecular complexes. Water trimer anion. Journal of Chemical Physics, 1997, 107, 5788-5793.	3.0	57
26	Experimental and theoreticalab initiostudy of the influence of N-methylation on the dipole-bound electron affinities of thymine and uracil. Journal of Chemical Physics, 1999, 110, 11876-11883.	3.0	57
27	Solving the singleâ€reference coupledâ€cluster equations involving highly excited clusters in quasidegenerate situations. Journal of Chemical Physics, 1994, 100, 5857-5869.	3.0	50
28	Lowest Excitation Energy of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mmultiscripts><mml:mi>Be</mml:mi><mml:mprescripts /><mml:none /><mml:mn>9</mml:mn></mml:mmultiscripts></mml:math>. Physical Review Letters, 2007, 99, 043001.	7.8	50
29	Experimental and ab initio theoretical studies of electron binding to formamide, N-methylformamide, and N,N-dimethylformamide. Journal of Chemical Physics, 1999, 110, 4309-4314.	3.0	49
30	Non-Born-Oppenheimer Isotope Effects on the Polarizabilities ofH2. Physical Review Letters, 2002, 89, 073001.	7.8	49
31	Theoretical investigations of proton transfer reactions in a hydrogen bonded complex of cytosine with water. Journal of Chemical Physics, 1995, 102, 5708-5718.	3.0	48
32	Matrix-Isolation FT-IR Studies andab InitioCalculations of Hydrogen-Bonded Complexes of Molecules Modeling Cytosine or Isocytosine Tautomers. 5. 1-CH3-Cytosine Complexes with H2O in Ar Matrices. The Journal of Physical Chemistry, 1996, 100, 6434-6444.	2.9	48
33	Nonadiabatic Calculations of the Dipole Moments of LiH and LiD. Physical Review Letters, 2002, 88, 033002.	7.8	48
34	Ab initio theoretical study of dipoleâ€“bound anions of molecular complexes: Water tetramer anions. Journal of Chemical Physics, 1998, 109, 1238-1244.	3.0	47
35	Dipole-Bound Anions of Adenineâ‹¯Water Clusters. Ab Initio Study. Journal of Physical Chemistry A, 2001, 105, 1033-1038.	2.5	47
36	Computed structure and energetics of La@C60. International Journal of Quantum Chemistry, 2005, 104, 272-277.	2.0	47

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37	Energy and energy gradient matrix elements with N-particle explicitly correlated complex Gaussian basis functions with L=1. Journal of Chemical Physics, 2008, 128, 114107.	3.0	47
38	High accuracy non-Bornâ€“Oppenheimer calculations for the isotopomers of the hydrogen molecule with explicitly correlated Gaussian functions. Journal of Chemical Physics, 2000, 113, 4203-4205.	3.0	46
39	Noncovalent Interaction of Methylene Blue with Carbon Nanotubes: Theoretical and Mass Spectrometry Characterization. Journal of Physical Chemistry C, 2012, 116, 20579-20590.	3.1	46
40	Structures and electron affinities of indoleâ€“(water)N clusters. Journal of Chemical Physics, 2000, 112, 3726-3734.	3.0	44
41	Ab initio characterization of electronically excited states in highly unsaturated hydrocarbons. Journal of Chemical Physics, 1995, 102, 394-399.	3.0	43
42	Nonrelativistic variational calculations of the positronium molecule and the positronium hydride. Physical Review A, 2006, 74, .	2.5	42
43	Matrix elements of N-particle explicitly correlated Gaussian basis functions with complex exponential parameters. Journal of Chemical Physics, 2006, 124, 224317.	3.0	41
44	Non-Bornâ€“Oppenheimer calculations of the BH molecule. Journal of Chemical Physics, 2009, 131, 044128.	3.0	41
45	High-accuracy calculations of the ground, 1â€‰A11â€², and the 2â€‰A11â€², 2â€‰A31â€², and 1â€‰E1â€² excited states of H3+. Journal of Chemical Physics, 2009, 130, 034104.	3.0	40
46	Combined Raman scattering and ab initio investigation of the interaction between pyrene and carbon SWNT. Molecular Physics, 2003, 101, 2609-2614.	1.7	39
47	Equivalent quantum approach to nuclei and electrons in molecules. Chemical Reviews, 1993, 93, 2007-2022.	47.7	37
48	Isomeric Sc₂O@C₇₈ Related by a Single-Step Stoneâ€“Wales Transformation: Key Links in an Unprecedented Fullerene Formation Pathway. Inorganic Chemistry, 2016, 55, 11354-11361.	4.0	37
49	Electron affinity of hydrogen, deuterium, and tritium: A nonadiabatic variational calculation using explicitly correlated Gaussian basis functions. Journal of Chemical Physics, 1997, 106, 4589-4595.	3.0	36
50	Gibbs energy-based treatment of metallofullerenes: Ca@C72, Ca@C74, Ca@C82, and La@C82. Molecular Simulation, 2005, 31, 71-77.	2.0	36
51	Electron affinities of small linear carbon clusters. Coupled cluster calculations with firstâ€order correlation orbitals. Journal of Chemical Physics, 1991, 94, 1241-1246.	3.0	35
52	C80, C86, C88: Semiempirical and ab initio SCF calculations. International Journal of Quantum Chemistry, 1997, 63, 529-535.	2.0	35
53	Non-Bornâ€“Oppenheimer calculations of the pure vibrational spectrum of HeH+. Journal of Chemical Physics, 2005, 123, 104306.	3.0	35
54	Dipoleâ€bound anionic state of nitromethane. Ab initio coupled cluster study with firstâ€order correlation orbitals. Journal of Chemical Physics, 1989, 91, 7787-7790.	3.0	34

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55	Stateâ€selective multiâ€reference coupledâ€cluster theory employing the singleâ€reference formalism: Application to an excited state of H8. Journal of Chemical Physics, 1995, 102, 3301-3306.	3.0	34
56	Non-Bornâ€“Oppenheimer calculations on the LiH molecule with explicitly correlated Gaussian functions. Journal of Chemical Physics, 2001, 114, 3393-3397.	3.0	34
57	Computing enthalpy-entropy interplay for isomeric fullerenes. International Journal of Quantum Chemistry, 2004, 99, 640-653.	2.0	34
58	New more accurate calculations of the ground state potential energy surface of H3+. Journal of Chemical Physics, 2009, 130, 074105.	3.0	34
59	Computed stabilities in metallofullerene series: Al@C₈₂, Sc@C₈₂, Y@C₈₂, and La@C₈₂. International Journal of Quantum Chemistry, 2011, 111, 2712-2718.	2.0	34
60	H-Bonded and Stacked Dimers of Pyrimidine and p-Benzoquinone. A Combined Matrix Isolation Infrared and Theoretical ab Initio Study. Journal of Physical Chemistry A, 1997, 101, 7208-7216.	2.5	33
61	Matrix-Isolation FT-IR Study and Theoretical Calculations of the Hydrogen-Bond Interaction of Hypoxanthine with H2O. Journal of Physical Chemistry A, 2002, 106, 4502-4512.	2.5	33
62	Implementation of analytical first derivatives for evaluation of the manyâ€body nonadiabatic wave function with explicitly correlated Gaussian functions. Journal of Chemical Physics, 1992, 96, 9013-9024.	3.0	32
63	Ab initio theoretical study of dipoleâ€“bound anions of molecular complexes:â€‚Water pentamer anions. Journal of Chemical Physics, 1999, 110, 3804-3810.	3.0	32
64	State-specific multireference complete-active-space coupled-cluster approach versus other quantum chemical methods: dissociation of the N₂molecule. Molecular Physics, 2007, 105, 1335-1357.	1.7	32
65	Out-of-plane vibrations of NH2 in 2-aminopyrimidine and formamide. Journal of Chemical Physics, 1998, 108, 10116-10128.	3.0	31
66	Dissociation of the fluorine molecule: CASCCSD method and other many-particle models. International Journal of Quantum Chemistry, 2006, 106, 2875-2880.	2.0	31
67	Lower Rydberg<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup><mml:mi>D</mml:mi></mml:mrow></mml:math>states of the lithium atom: Finite-nuclear-mass calculations with explicitly correlated Gaussian functions.	2.5	31
68	Algorithm for quantum-mechanical finite-nuclear-mass variational calculations of atoms with two<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>electrons using all-electron explicitly correlated Gaussian basis functions. Physical Review A, 2009, 80, .	2.5	30
69	Analytical energy gradient in variational calculations of the two lowest P3 states of the carbon atom with explicitly correlated Gaussian basis functions. Journal of Chemical Physics, 2010, 132, 184106.	3.0	30
70	Is the C8ring nonplanar?. Molecular Physics, 1992, 76, 387-393.	1.7	29
71	One-, Two- and Three-Dimensional Structures of C20. Fullerenes, Nanotubes, and Carbon Nanostructures, 1993, 1, 1-9.	0.6	28
72	Non-Bornâ€“Oppenheimer calculations of the polarizability of LiH in a basis of explicitly correlated Gaussian functions. Journal of Chemical Physics, 2002, 116, 5557-5564.	3.0	28

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73	Accuracy limits on the description of the lowest<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>S</mml:mi></mml:math>excitation in the Li atom using explicitly correlated Gaussian basis functions. Physical Review A, 2008, 78, .	2.5	28
74	The electronic and geometrical structure of aluminum fluoride anions AlFâ¯n,n=1â€“4, and electron affinity of their neutral parents. Journal of Chemical Physics, 1994, 100, 8925-8933.	3.0	27
75	Computing fullerene encapsulation of non-metallic molecules: N2@C60and NH3@C60. Molecular Simulation, 2005, 31, 801-806.	2.0	27
76	Isotope shifts of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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91	Multicenter and multiparticle integrals for explicitly correlated cartesian gaussian-type functions. Journal of Computational Chemistry, 1992, 13, 602-613.	3.3	22
92	Methylation Reduces Electron Affinity of Uracil. Ab Initio Theoretical Study. Journal of Physical Chemistry A, 1997, 101, 8123-8127.	2.5	22
93	Matrix-Isolation FT-IR Studies and ab Initio Calculations of Hydrogen-Bonded Complexes of Molecules Modeling Cytosine or Isocytosine Tautomers. 6. Experimental Observation of a Water-Induced Tautomeric Shift for 2-Hydroxypyrimidine and 5-Bromo-2-hydroxypyrimidine. Journal of Physical Chemistry A, 1998, 102, 8157-8168.	2.5	22
94	Noncovalent Interaction of Graphene with Heterocyclic Compounds: Benzene, Imidazole, Tetracene, and Imidazophenazines. ChemPhysChem, 2016, 17, 1204-1212.	2.1	22
95	The structure of the CFâˆ’4 anion and the electron affinity of the CF4 molecule. Journal of Chemical Physics, 1995, 102, 9309-9314.	3.0	21
96	A Dynamic Model for Electron Transport in DNA. Journal of Physical Chemistry B, 2001, 105, 9345-9354.	2.6	21
97	Relativistic corrections to the ground-state energy of the positronium molecule. Physical Review A, 2007, 75, .	2.5	21
98	Fundamental vibrational transitions of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mmultiscripts><mml:mtext>H</mml:mtext><mml:mprescripts /><mml:none /><mml:mn>3</mml:mn></mml:mmultiscripts><mml:mtext>e</mml:mtext><mml:mtext>â€‰</mml:mtext><mml:msup><mml:mrow /><mml:none /><mml:mn>4</mml:mn></mml:mmultiscripts><mml:mtext>e</mml:mtext></mml:mrow><mm	2.5	21
99	Ab initio theoretical study of dipole-bound anions of molecular complexes: (HF)3â¯ and (HF)4â¯ anions. Journal of Chemical Physics, 1997, 107, 9475-9481.	3.0	20
100	Two Uracil Molecules Connected by an Excess Electron. Journal of Physical Chemistry A, 2002, 106, 6099-6101.	2.5	20
101	Three lowest<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>S</mml:mi></mml:math>states of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mmultiscripts><mml:mtext>B</mml:mtext><mml:mprescripts /><mml:none /><mml:mn>9</mml:mn></mml:mmultiscripts><mml:mtext>e</mml:mtext></mml:mrow><mml:mo>+</mml:mo></mml:msup></mml:mr	2.5	20
102	Impact of Local Curvature and Structural Defects on Grapheneâ€“C₆₀ Fullerene Fusion Reaction Barriers. Journal of Physical Chemistry C, 2013, 117, 19664-19671.	3.1	20
103	Conformational composition of neutral leucine. Matrix isolation infrared and ab initio study. Chemical Physics, 2013, 423, 20-29.	1.9	20
104	Microwave measurements and theoretical calculations on the structures of NNOâ€“HCl complexes. Journal of Chemical Physics, 1991, 94, 899-907.	3.0	19
105	AnAb InitioStudy of the Isomerization of Mgâˆ’ and Caâˆ’Pyrophosphates. Journal of the American Chemical Society, 1998, 120, 6113-6120.	13.7	19
106	New scheme for solving the amplitude equations in the state-specific coupled cluster theory with complete active space reference for ground and excited states. Journal of Chemical Physics, 2000, 113, 8503-8513.	3.0	19
107	New indices for describing the multi-configurational nature of the coupled cluster wave function. Molecular Physics, 2005, 103, 2131-2139.	1.7	19
108	Lowest vibrational states ofHe4He+3: Non-Born-Oppenheimer calculations. Physical Review A, 2007, 76, .	2.5	19

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109	Calculations of low-lying<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mmultiscripts><mml:mi>P</mml:mi><mml:mprescripts /><mml:none /><mml:mn>1</mml:mn></mml:mmultiscripts></mml:math>states of the beryllium atom. Physical Review A, 2009, 79, .	2.5	19
110	p-Quinone Dimers:Â H-Bonding vs Stacked Interaction. Matrix-Isolation Infrared and ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 11052-11059.	2.5	18
111	Normal mode analysis of the vibrational spectrum of tropolone-A molecule with seven-membered ring. International Journal of Quantum Chemistry, 2002, 90, 1163-1173.	2.0	18
112	Darwin and mass-velocity relativistic corrections in the non-Born-Oppenheimer calculations of pure vibrational states of H2. Journal of Chemical Physics, 2006, 125, 014318.	3.0	18
113	Computed structures and relative stabilities of Be@C74. International Journal of Quantum Chemistry, 2007, 107, 2494-2498.	2.0	18
114	Accurate Bornâ€“Oppenheimer calculations of the lowâ€lying c³Îž and a³Îž excited states of helium dimer. International Journal of Quantum Chemistry, 2008, 108, 2291-2298.	2.0	18
115	Accurate one-dimensional potential energy curve of the linear (H2)2 cluster. Journal of Chemical Physics, 2010, 133, 124106.	3.0	18
116	Progress in calculating the potential energy surface of H ₃ ⁺. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 5001-5013.	3.4	18
117	An algorithm for non-Born-Oppenheimer quantum mechanical variational calculations of N = 1 rotationally excited states of diatomic molecules using all-particle explicitly correlated Gaussian functions. Journal of Chemical Physics, 2013, 139, 164119.	3.0	18
118	Binding of Polycitydylic Acid to Graphene Oxide: Spectroscopic Study and Computer Modeling. Journal of Physical Chemistry C, 2017, 121, 18221-18233.	3.1	18
119	Ground and excited <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mmultiscripts><mml:mi>S</mml:mi><mml:mprescripts /><mml:none /><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:mmultiscripts></mml:mrow></mml:math> states of the beryllium atom. Physical Review A, 2010, 109, .	2.5	18
120	Firstâ€order correlation orbitals for the spinâ€unrestricted Hartreeâ€“Fock zeroâ€order wave function. Electron affinities of C4 clusters. Journal of Chemical Physics, 1990, 93, 6685-6693.	3.0	17
121	Application of explicitly correlated Gaussian functions for calculations of the ground state of the beryllium atom. Journal of Computational Chemistry, 1993, 14, 566-570.	3.3	17
122	Dipole-Bound Anions to Adenineâ^'Imidazole Complex. Ab Initio Study. Journal of Physical Chemistry A, 2001, 105, 1071-1073.	2.5	17
123	Complete<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi>Î±</mml:mi><mml:mn>2</mml:mn></mml:msup></mml:mrow></mml:math>relativistic corrections to the pure vibrational non-Born-Oppenheimer energies of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mtext>HeH</mml:mtext></mml:mrow><mml:mo>+</mml:mo></mml:msup></mml:mrow></mml:math> ions. Physical Review A, 2008, 77, .	2.5	17
124	An algorithm for nonrelativistic quantum-mechanical finite-nuclear-mass variational calculations of nitrogen atom in L = 0, M = 0 states using all-electrons explicitly correlated Gaussian basis functions. Journal of Chemical Physics, 2014, 140, 174112.	3.0	17
125	Theoretical study of doubly charged negative ions of elemental clusters. Stability of C2â^'8. Journal of Chemical Physics, 1991, 95, 8669-8670.	3.0	16
126	Excited electronic states and relative stabilities of C80 isomers. International Journal of Quantum Chemistry, 2006, 106, 2222-2228.	2.0	16

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127	Computations on three isomers of La@C₇₄. International Journal of Quantum Chemistry, 2008, 108, 2636-2640.	2.0	16
128	Optimized virtual orbital space (OVOS) in coupled-cluster calculations. Molecular Physics, 2010, 108, 3105-3112.	1.7	16
129	Accurate potential energy curves for HeH+ isotopologues. Journal of Chemical Physics, 2012, 137, 164305.	3.0	16
130	Communication: Visible line intensities of the triatomic hydrogen ion from experiment and theory. Journal of Chemical Physics, 2014, 141, 241104.	3.0	16
131	Anharmonic contributions to the inversion vibration in 2â€aminopyrimidine. Journal of Chemical Physics, 1995, 103, 656-662.	3.0	15
132	Isomerism of the Covalent Anion of the Uracilâ^'Thymine Dimer. Ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 4309-4312.	2.5	15
133	Integrals for non-Bornâ€“Oppenheimer calculations of molecules with three nuclei. Molecular Physics, 2005, 103, 1169-1182.	1.7	15
134	Improved calculations of the lowest vibrational transitions inHeH+. Physical Review A, 2007, 76, .	2.5	15
135	Non-Born-Oppenheimer calculations of the lowest vibrational energy of HD including relativistic corrections. Physical Review A, 2009, 79, .	2.5	15
136	Chloromethane and dichloromethane decompositions inside nanotubes as models of reactions in confined space. Theoretical Chemistry Accounts, 2009, 124, 95-103.	1.4	15
137	Explicitly correlated Gaussian calculations of the 2P o Rydberg spectrum of the lithium atom. Journal of Chemical Physics, 2012, 136, 134305.	3.0	15
138	Calculations of the water-dimer encapsulations into C84. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 1-7.	2.1	15
139	Calculated relative yields for Sc2S@C82 and Y2S@C82. Theoretical Chemistry Accounts, 2011, 130, 549-554.	1.4	14
140	Evaluation of the relative stabilities of two non-IPR isomers of Sm@C76. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 339-344.	2.1	14
141	A computational characterization of CO@C₆₀. Fullerenes Nanotubes and Carbon Nanostructures, 2017, 25, 624-629.	2.1	14
142	Simultaneous optimization of molecular geometry and the wave function in a basis of Singer's n-electron explicitly correlated Gaussians. Chemical Physics Letters, 2001, 335, 404-408.	2.6	13
143	Electronic excited states and stabilities of fullerenes: Isomers of C78and Mg@C72. International Journal of Quantum Chemistry, 2004, 100, 610-616.	2.0	13
144	An algorithm for quantum mechanical finite-nuclear-mass variational calculations of atoms with L = 3 using all-electron explicitly correlated Gaussian basis functions. Journal of Chemical Physics, 2013, 138, 104107.	3.0	13

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145	Algorithms for calculating mass-velocity and Darwin relativistic corrections with n-electron explicitly correlated Gaussians with shifted centers. Journal of Chemical Physics, 2016, 144, 174101.	3.0	13
146	Calculated relative populations of Sm@C₈₂ isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2018, 26, 233-238.	2.1	13
147	A new N-body potential and basis set for adiabatic and non-adiabatic variational energy calculations. Journal of Chemical Physics, 1997, 106, 8760-8768.	3.0	12
148	Competition between H-bonded and stacked dimers of pyrimidine: IR and theoretical ab-initio study. Molecular Physics, 1997, 91, 513-526.	1.7	12
149	Quantum-Chemical Calculations of Model Systems of Interest in Fullerene-Based Superconductivity. Journal of Low Temperature Physics, 2003, 131, 1259-1263.	1.4	12
150	Computed Relative Populations of D₂(22)â€Œ₈₄ Endohedrals with Encapsulated Monomeric and Dimeric Water. ChemPhysChem, 2016, 17, 1109-1111.	2.1	12
151	Benchmark Rovibrational Linelists and Einstein A-coefficients for the Primordial Molecules and Isotopologues. Astrophysical Journal, 2019, 878, 95.	4.5	12
152	Computer program ATOM-MOL-nonBO for performing calculations of ground and excited states of atoms and molecules without assuming the Bornâ€“Oppenheimer approximation using all-particle complex explicitly correlated Gaussian functions. Journal of Chemical Physics, 2020, 152, 204102.	3.0	12
153	A CASSCF-CASPT2 study of the excited-state intramolecular proton transfer reaction in 1-amino-3-propenal using different active spaces. Journal of Computational Chemistry, 1999, 20, 1422-1431.	3.3	11
154	Theoretical characterization of intramolecular proton transfer in the ground and the lowest-lying triplet excited states of 1-amino-3-propenal: a methodological comparison. Journal of Computational Chemistry, 2000, 21, 257-269.	3.3	11
155	Analytical gradients for Singer's multicentern-electron explicitly correlated Gaussians. International Journal of Quantum Chemistry, 2001, 82, 151-159.	2.0	11
156	Stability calculations for Eu@C₇₄ isomers. International Journal of Quantum Chemistry, 2013, 113, 729-733.	2.0	11
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