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 computational characterization of H₂O₂@C₆₀. Fullerenes Nanotubes and Carbon Nanostructures, 2022, 30, 258-262.	2.1	2
2	Fine structure of the beryllium <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mmultiscripts><mml:mi>P</mml:mi><mml:mprescripts /><mml:none /><mml:mn>3</mml:mn></mml:mmultiscripts></mml:math> states calculated with all-electron explicitly correlated Gaussian functions. Physical Review A, 2022, 105, .	2.5	1
3	Photoreactions of Sc3N@C80 with Disilirane, Silirane, and Digermirane: A Photochemical Method to Separate Ih and D5h Isomers. Photochem, 2022, 2, 122-137.	2.2	1
4	Electron affinity of LiH⁻. Molecular Physics, 2022, 120, .	1.7	1
5	Calculated relative populations for the Eu@C84 isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2021, 29, 144-148.	2.1	5
6	The influence of low-temperature argon matrix on embedded water clusters. A DFT theoretical study. Low Temperature Physics, 2021, 47, 242-249.	0.6	2
7	Coronene-uracil complexes embedded in argon matrices: FTIR spectroscopy and quantum-mechanical calculations. Low Temperature Physics, 2021, 47, 325-334.	0.6	0
8	High-accuracy calculations of the lowest eleven Rydberg 2 P states of the Li atom. Journal of Physics B: Atomic, Molecular and Optical Physics, 2021, 54, 085003.	1.5	4
9	Benchmark calculations of the 2D Rydberg spectrum of lithium. Molecular Physics, 2021, 119, e1925765.	1.7	1
10	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mmultiscripts><mml:mi>S</mml:mi><mml:mprescripts /><mml:none /><mml:mn>2</mml:mn></mml:mmultiscripts></mml:math> Rydberg spectrum of the boron atom. Physical Review A, 2021, 104, .	2.5	7
11	Benchmark Calculations of the Energy Spectra and Oscillator Strengths of the Beryllium Atom. Journal of Physical and Chemical Reference Data, 2021, 50, .	4.2	4
12	Modeling of nucleobase/oligonucleotide interaction with graphene and graphene oxide: the role of charging and/or oxidizing the graphene surface. Molecular Crystals and Liquid Crystals, 2020, 697, 49-59.	0.9	1
13	Adsorption of Polyadenylic acid on graphene oxide: experiments and computer modeling. Journal of Biomolecular Structure and Dynamics, 2020, , 1-13.	3.5	2
14	Electronic perturbation effects in the presence of electric field for <scp>Ï€â€conjugated</scp> systems: An electronâ€correlation study. International Journal of Quantum Chemistry, 2020, 120, e26260.	2.0	1
15	Treating the motion of nuclei and electrons in atomic and molecular quantum mechanical calculations on an equal footing: Non-Bornâ€“Oppenheimer quantum chemistry. Advances in Quantum Chemistry, 2020, 81, 143-166.	0.8	5
16	Low-temperature sensibilization of naphthalene phosphorescence using ortho-bromobenzophenone. Low Temperature Physics, 2020, 46, 71-77.	0.6	0
17	Eu@C86 isomers: Calculated relative populations. Fullerenes Nanotubes and Carbon Nanostructures, 2020, 28, 565-570.	2.1	7
18	The effect of matrices on the low-temperature IR spectra of a formic acid molecule isolated in inert gas crystals. Low Temperature Physics, 2020, 46, 155-164.	0.6	2

#	Article	IF	Citations
19	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
20	Low-lying <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mmultiscripts><mml:mi>S</mml:mi><mml:mprescripts /><mml:none /><mml:mn>2</mml:mn></mml:mmultiscripts></mml:math> states of the singly charged carbon ion. Physical Review A, 2020, 102, .	2.5	8
21	Non-adiabatic effects in the H ₃ ⁺ spectrum. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180411.	3.4	4
22	Lowest ten ¹ P Rydberg states of beryllium calculated with all-electron explicitly correlated Gaussian functions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2019, 52, 155002.	1.5	7
23	Calculations of the relative populations of Lu@C₈₂ isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2019, 27, 710-714.	2.1	10
24	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, 2019, 100, .	2.5	18
25	Implementation of explicitly correlated complex Gaussian functions in calculations of molecular rovibrational <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si7.gif" overflow="scroll"><mml:mrow><mml:mi>J</mml:mi><mml:mo>=</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:math> states without Born-Oppenheimer approximation. Chemical Physics Letters, 2019, 717, 147-151.	2.6	4
26	Benchmark Rovibrational Linelists and Einstein A-coefficients for the Primordial Molecules and Isotopologues. Astrophysical Journal, 2019, 878, 95.	4.5	12
27	Theoretical modeling of DNA electron hole transport through polypyrimidine sequences: a QM/MM study. Journal of Molecular Modeling, 2019, 25, 97.	1.8	1
28	Interaction of Single Walled Carbon Nanotube with Graphene: Quantum-Chemical Calculation and Molecular Dynamics Study. , 2019, , .		0
29	Finite-nuclear-mass calculations of the leading relativistic corrections for atomic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>D</mml:mi></mml:math> states with all-electron explicitly correlated Gaussian functions. Physical Review A, 2019, 100, .	2.5	7
30	Calculations of the Lu₃N@C₈₀ two-isomer equilibrium. Fullerenes Nanotubes and Carbon Nanostructures, 2019, 27, 382-386.	2.1	6
31	Calculated relative populations of Sm@C₈₂ isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2018, 26, 233-238.	2.1	13
32	Leading relativistic corrections for atomicPstates calculated with a finite-nuclear-mass approach and all-electron explicitly correlated Gaussian functions. Physical Review A, 2018, 97, .	2.5	6
33	A computational quantum-mechanical model of a molecular magnetic trap. Journal of Chemical Physics, 2018, 149, 244112.	3.0	6
34	Lowest<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mmultiscripts><mml:mrow><mml:mi>S</mml:mi></mml:mrow><mml:mprescripts /><mml:none /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:mmultiscripts></mml:mrow></mml:math>Electronic Excitations of the Boron Atom. Physical Review Letters, 2017, 118, 043001.	7.8	11
35	Explicitly-correlated non-born-oppenheimer calculations of the HD molecule in a strong magnetic field. Chemical Physics Letters, 2017, 682, 87-90.	2.6	7
36	Non-Born-Oppenheimer calculations of the rovibrational spectrum of H2 excited to the second rotational level. Chemical Physics Letters, 2017, 669, 188-191.	2.6	5

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37	Binding of Polycitydylic Acid to Graphene Oxide: Spectroscopic Study and Computer Modeling. Journal of Physical Chemistry C, 2017, 121, 18221-18233.	3.1	18
38	A computational characterization of CO@C₆₀. Fullerenes Nanotubes and Carbon Nanostructures, 2017, 25, 624-629.	2.1	14
39	L₁-regularisation of the coupled-cluster solutions. Molecular Physics, 2017, 115, 2892-2902.	1.7	1
40	Stability issues in computational screening of carbon nanostructures: illustrations on La endohedrals. Molecular Simulation, 2017, 43, 1472-1479.	2.0	8
41	Relativistic corrections for non-Born-Oppenheimer molecular wave functions expanded in terms of complex explicitly correlated Gaussian functions. Physical Review A, 2017, 95, .	2.5	4
42	Algorithms for calculating the leading quantum electrodynamics P(1/r 3) correction with all-electron molecular explicitly correlated Gaussians. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 065101.	1.5	7
43	Sc₂O@C₇₈: Calculations of the yield ratio for two observed isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2017, 25, 124-127.	2.1	10
44	Eu@C72: Computed Comparable Populations of Two Non-IPR Isomers. Molecules, 2017, 22, 1053.	3.8	25
45	Statistical Contact Model for Confined Molecules. Journal of Statistical Physics, 2016, 164, 1000-1025.	1.2	7
46	Noncovalent Interaction of Graphene with Heterocyclic Compounds: Benzene, Imidazole, Tetracene, and Imidazophenazines. ChemPhysChem, 2016, 17, 1204-1212.	2.1	22
47	Computed Relative Populations of D₂(22)â€Œ₈₄ Endohedrals with Encapsulated Monomeric and Dimeric Water. ChemPhysChem, 2016, 17, 1109-1111.	2.1	12
48	Computational and photoelectron spectroscopic study of the dipole-bound anions, indole(H2O)1,2â^'. Journal of Chemical Physics, 2016, 145, 024301.	3.0	10
49	Orbit-orbit relativistic correction calculated with all-electron molecular explicitly correlated Gaussians. Journal of Chemical Physics, 2016, 145, 224111.	3.0	5
50	Charge asymmetry and rovibrational excitations of HD⁺. Molecular Physics, 2016, 114, 2052-2073.	1.7	3
51	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
52	The effect of protonation of cytosine and adenine on their interactions with carbon nanotubes. Journal of Molecular Graphics and Modelling, 2016, 70, 77-84.	2.4	10
53	Effect of low-temperature argon matrices on the IR spectra and structure of flexible N-acetylglycine molecules. Low Temperature Physics, 2016, 42, 1167-1174.	0.6	4
54	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

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55	Nuclearâ€“nuclear correlation function from non-Bornâ€“Oppenheimer calculations of diatomic rovibrational states with total angular momentum equal to two (N = 2). Charge asymmetry in HD. Molecular Physics, 2016, 114, 1634-1643.	1.7	3
56	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
57	Universal all-particle explicitly-correlated Gaussians for non-Bornâ€“Oppenheimer calculations of molecular rotationless states. Chemical Physics Letters, 2016, 647, 122-126.	2.6	11
58	Accurate dipole moment curve and non-adiabatic effects on the high resolution spectroscopic properties of the LiH molecule. Journal of Molecular Spectroscopy, 2016, 322, 22-28.	1.2	9
59	Calculations of the water-dimer encapsulations into C84. Fullerenes Nanotubes and Carbon Nanostructures, 2016, 24, 1-7.	2.1	15
60	Non-Bornâ€“Oppenheimer variational method for calculation of rotationally excited binuclear systems. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 195101.	1.5	8
61	Connecting a new non-adiabatic vibrational mass to the bonding mechanism of LiH: A quantum superposition of ionic and covalent states. Chemical Physics Letters, 2015, 633, 89-94.	2.6	6
62	Direct non-Born-Oppenheimer variational calculations of all bound vibrational states corresponding to the first rotational excitation of D2 performed with explicitly correlated all-particle Gaussian functions. Journal of Chemical Physics, 2015, 142, 174307.	3.0	1
63	Non-Bornâ€“Oppenheimer calculations of the HD molecule in a strong magnetic field. Chemical Physics Letters, 2015, 639, 295-299.	2.6	10
64	Discontinuities-free complete-active-space stateâ€“specific multiâ€“reference coupled cluster theory for describing bond stretching and dissociation. Journal of Chemical Physics, 2015, 143, 024109.	3.0	6
65	Microscopic pressure-cooker model for studying molecules in confinement. Molecular Physics, 2015, 113, 671-682.	1.7	7
66	Sm@C74: Computed Relative Isomeric Populations. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 235-242.	2.1	3
67	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
68	Accurate potential energy curve of the LiH+ molecule calculated with explicitly correlated Gaussian functions. Journal of Chemical Physics, 2014, 140, 124315.	3.0	7
69	Prediction of1PRydberg energy levels of beryllium based on calculations with explicitly correlated Gaussians. Journal of Chemical Physics, 2014, 140, 024301.	3.0	5
70	A comparison of two types of explicitly correlated Gaussian functions for non-Born-Oppenheimer molecular calculations using a model potential. Journal of Chemical Physics, 2014, 141, 154103.	3.0	7
71	Accurate non-Born-Oppenheimer calculations of the complete pure vibrational spectrum of dititium using all-particle explicitly correlated Gaussian functions. Journal of Chemical Physics, 2014, 140, .	3.0	4
72	Charge asymmetry in the rovibrationally excited HD molecule. Journal of Chemical Physics, 2014, 140, 104115.	3.0	6

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73	Non-Born-Oppenheimer calculations of the pure vibrational spectrum of T2 including relativistic corrections. Journal of Chemical Physics, 2014, 141, 154302.	3.0	3
74	Charge asymmetry and relativistic corrections in pure vibrational states of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>HD</mml:mi><mml:mo>+</mml:mo></mml:msup></mml Physical Review A, 2014, 89, .	2.5	5
75	Lifetimes of rovibrational levels ofHD+. Physical Review A, 2014, 89, .	2.5	3
76	Lower Rydberg2Fstates of the lithium atom: finite-nuclear-mass calculations with explicitly correlated Gaussian functions. Molecular Physics, 2014, 112, 805-808.	1.7	2
77	Computations on Metallofullerenes Derivatized during Extraction: La@C80-C6H3Cl2 and La@C82-C6H3Cl2. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 173-181.	2.1	5
78	Towards Relative Populations of Non-Isomeric Metallofullerenes: La@C76( ) vs. La2@C76(,17490). Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 299-306.	2.1	7
79	Unusual behavior of the pyrimidineâ€“2-hydroxypyrimidine heterodimer isolated in argon matrices. Chemical Physics Letters, 2014, 608, 84-89.	2.6	2
80	Communication: Visible line intensities of the triatomic hydrogen ion from experiment and theory. Journal of Chemical Physics, 2014, 141, 241104.	3.0	16
81	Stability calculations for Eu@C₇₄ isomers. International Journal of Quantum Chemistry, 2013, 113, 729-733.	2.0	11
82	Selection of a Gaussian basis set for calculating the Bethe logarithm for the ground state of the hydrogen atom. Molecular Physics, 2013, 111, 1063-1068.	1.7	4
83	Prediction of2SRydberg energy levels of6Li and7Li based on quantum-mechanical calculations performed with explicitly correlated Gaussian functions. Physical Review A, 2013, 87, .	2.5	4
84	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
85	Conformational composition of neutral leucine. Matrix isolation infrared and ab initio study. Chemical Physics, 2013, 423, 20-29.	1.9	20
86	Molecular dipole static polarisabilities and hyperpolarisabilities of conjugated oligomer chains calculated with the local ï€-electron coupled cluster theory. Molecular Physics, 2013, 111, 3779-3792.	1.7	7
87	Theory and application of explicitly correlated Gaussians. Reviews of Modern Physics, 2013, 85, 693-749.	45.6	263
88	Bornâ€“Oppenheimer and Non-Bornâ€“Oppenheimer, Atomic and Molecular Calculations with Explicitly Correlated Gaussians. Chemical Reviews, 2013, 113, 36-79.	47.7	129
89	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
90	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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91	Non-Born-Oppenheimer method for direct variational calculations of diatomic first excited rotational states using explicitly correlated all-particle Gaussian functions. Physical Review A, 2013, 88, .	2.5	9
92	Assessment of the accuracy the experimental energies of the1Po1s22s6pand 1s22s7pstates of9Be based on variational calculations with explicitly correlated Gaussians. Journal of Chemical Physics, 2012, 137, 104315.	3.0	5
93	Explicitly correlated Gaussian calculations of the 2P o Rydberg spectrum of the lithium atom. Journal of Chemical Physics, 2012, 136, 134305.	3.0	15
94	Accurate potential energy curves for HeH+ isotopologues. Journal of Chemical Physics, 2012, 137, 164305.	3.0	16
95	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
96	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
97	State-specific multireference coupled-cluster theory of molecular electronic excited states. Annual Reports on the Progress of Chemistry Section C, 2011, 107, 169.	4.4	8
98	Exponentially and pre-exponentially correlated Gaussians for atomic quantum calculations. Journal of Chemical Physics, 2011, 134, 094104.	3.0	5
99	Calculated relative yields for Sc2S@C82 and Y2S@C82. Theoretical Chemistry Accounts, 2011, 130, 549-554.	1.4	14
100	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
101	Accurate variational calculations of the ground 2P o(1s22s22p) and excited 2S(1s22s2p2) and 2P o(1s22s23p) states of singly ionized carbon atom. Journal of Chemical Physics, 2011, 135, 214104.	3.0	10
102	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow /><mml:mn>1</mml:mn></mml:msup><mml:mi>D</mml:mi></mml:mrow></mml:math>states of the beryllium atom: Quantum mechanical nonrelativistic calculations employing explicitly correlated Gaussian functions. Physical Review A, 2011, 84, .	2.5	6
103	Complete pure vibrational spectrum of HD calculated without the Born-Oppenheimer approximation and including relativistic corrections. Physical Review A, 2011, 83, .	2.5	7
104	Correlated-Gaussian calculations of the ground and low-lying excited states of the boron atom. Physical Review A, 2011, 83, .	2.5	24
105	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. Physical Review A, 2011, 83, .	2.5	31
106	Competition between counterions and active protein sites to bind bisquaternary ammonium groups. A combined mass spectrometry and quantum chemistry model study. European Physical Journal D, 2010, 58, 287-296.	1.3	8
107	Ionized states of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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109	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
110	Raman Spectroscopy and Theoretical Characterization of Nanohybrids of Porphyrins with Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 16215-16222.	3.1	24
111	Accurate one-dimensional potential energy curve of the linear (H2)2 cluster. Journal of Chemical Physics, 2010, 133, 124106.	3.0	18
112	Optimized virtual orbital space (OVOS) in coupled-cluster calculations. Molecular Physics, 2010, 108, 3105-3112.	1.7	16
113	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:mrow /></mml:msup></mml:mrow></mml:math>	2.5	21
114	Non-Bornâ€“Oppenheimer calculations of the BH molecule. Journal of Chemical Physics, 2009, 131, 044128.	3.0	41
115	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
116	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
117	Non-Born-Oppenheimer calculations of the lowest vibrational energy of HD including relativistic corrections. Physical Review A, 2009, 79, .	2.5	15
118	New more accurate calculations of the ground state potential energy surface of H3+. Journal of Chemical Physics, 2009, 130, 074105.	3.0	34
119	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
120	Chloromethane and dichloromethane decompositions inside nanotubes as models of reactions in confined space. Theoretical Chemistry Accounts, 2009, 124, 95-103.	1.4	15
121	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
122	The hydroxyacetone (CH₃COCH₂(OH)) torsional potential and isomerization: A theoretical study. International Journal of Quantum Chemistry, 2008, 108, 279-288.	2.0	4
123	Computations on three isomers of La@C₇₄. International Journal of Quantum Chemistry, 2008, 108, 2636-2640.	2.0	16
124	Accurate Bornâ€“Oppenheimer calculations of the lowâ€lying c³Îź and a³Îź excited states of helium dimer. International Journal of Quantum Chemistry, 2008, 108, 2291-2298.	2.0	18
125	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
126	Computational screening of metallofullerenes for nanoscience: Sr@C₇₄. Molecular Simulation, 2008, 34, 17-21.	2.0	7

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127	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	2.5	20
128	Complete<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi>l±</mml:mi><mml:mn>2</mml:mn></mml:msup></mml:mrow></mml:math>relati 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:ms	2.5	17
129	Accurate Ritz-type 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
130	Alkali-metal clusters encapsulated into fullerenes: Computations on Lix@C60. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 541-547.	0.2	0
131	Ionization potential ofBe9calculated including nuclear motion and relativistic corrections. Physical Review A, 2007, 75, .	2.5	23
132	Computations of production yields for Ba@C₇₄ and Yb@C₇₄. Molecular Simulation, 2007, 33, 563-568.	2.0	7
133	Lowest vibrational states ofHe4He+3: Non-Born-Oppenheimer calculations. Physical Review A, 2007, 76, .	2.5	19
134	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
135	Improved calculations of the lowest vibrational transitions inHeH+. Physical Review A, 2007, 76, .	2.5	15
136	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
137	Stabilization of an excess electron on molecular surfaces by a pair of water molecules. Molecular Physics, 2007, 105, 925-932.	1.7	4
138	Relativistic corrections to the ground-state energy of the positronium molecule. Physical Review A, 2007, 75, .	2.5	21
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