Maciej Gutowski

List of Publications by Year
in descending order

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161 papers	9,457 citations	31976 53 h-index	40979 93 g-index
166 all docs	166 docs citations	166 times ranked	6842 citing authors

#	Article	IF	Citations
1	Non-linear and non-local behaviour in spontaneously electrical solids. Physical Chemistry Chemical Physics, 2018, 20, 5112-5116.	2.8	9
2	Assigning a structural motif using spontaneous molecular dipole orientation in thin films. Physical Chemistry Chemical Physics, 2018, 20, 29038-29044.	2.8	9
3	Electrophilicity of oxalic acid monomer is enhanced in the dimer by intermolecular proton transfer. Physical Chemistry Chemical Physics, 2017, 19, 29760-29766.	2.8	3
4	Different Conformations of 2â€²-Deoxycytidine in the Gas and Solid Phases: Competition between Intra- and Intermolecular Hydrogen Bonds. Journal of Physical Chemistry A, 2016, 120, 8199-8210.	2.5	12
5	A Comparative Study of Methanol Adsorption and Dissociation over WO3(001) and ReO3(001). Topics in Catalysis, 2015, 58, 655-664.	2.8	6
6	Importance of Time Scale and Local Environment in Electron-Driven Proton Transfer. The Anion of Acetoacetic Acid. Journal of the American Chemical Society, 2015, 137, 14329-14340.	13.7	11
7	Communication: Remarkable electrophilicity of the oxalic acid monomer: An anion photoelectron spectroscopy and theoretical study. Journal of Chemical Physics, 2014, 140, 221103.	3.0	12
8	Intermolecular Interactions between Molecules in Various Conformational States: The Dimer of Oxalic Acid. Journal of Physical Chemistry A, 2014, 118, 7385-7391.	2.5	11
9	Discovery of Most Stable Structures of Neutral and Anionic Phenylalanine through Automated Scanning of Tautomeric and Conformational Spaces. Journal of Chemical Theory and Computation, 2013, 9, 4374-4381.	5.3	5
10	Influence of Prototropic Reactions on the Absorption and Fluorescence Spectra of Methyl p-dimethylaminobenzoate and Its Two Ortho Derivatives. Journal of Fluorescence, 2011, 21, 1749-1762.	2.5	12
11	SSC: A tool for constructing libraries for systematic screening of conformers. Journal of Computational Chemistry, 2011, 32, 2047-2054.	3.3	7
12	Is Electronegativity a Useful Descriptor for the Pseudoâ€Alkali Metal NH₄?. Chemistry - A European Journal, 2011, 17, 13197-13205.	3.3	16
13	Reactivity of hydrogen and methanol on (001) surfaces of WO3, ReO3, WO3/ReO3 and ReO3/WO3. Catalysis Today, 2011, 165, 41-48.	4.4	31
14	Combinatorialâ€“computationalâ€“chemoinformatics (C3) approach to finding and analyzing low-energy tautomers. Journal of Computer-Aided Molecular Design, 2010, 24, 627-638.	2.9	12
15	Barrier-free proton transfer induced by electron attachment to the complexes between 1â€methylcytosine and formic acid. Molecular Physics, 2010, 108, 2621-2631.	1.7	7
16	Theoretical Investigations on the Formation and Dehydrogenation Reaction Pathways of H(NH₂BH₂)_nH (n = 1â^’4) Oligomers: Importance of Dihydrogen Interactions. Inorganic Chemistry, 2010, 49, 7710-7720.	4.0	38
17	The Anionic (9-Methyladenine)â^’(1-Methylthymine) Base Pair Solvated by Formic Acid. A Computational and Photoelectron Spectroscopy Study. Journal of Physical Chemistry B, 2010, 114, 11353-11362.	2.6	8
18	Ammoniaâ^’Hydrogen Bromide and Ammoniaâ^’Hydrogen Iodide Complexes: Anion Photoelectron and ab Initio Studies. Journal of Physical Chemistry A, 2010, 114, 1357-1363.	2.5	15

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19	Structure and Stability of Hydrogen Clathrates of Ammonia Borane. Materials Research Society Symposia Proceedings, 2009, 1216, 1.	0.1	1
20	Comparison of some representative density functional theory and wave function theory methods for the studies of amino acids. Journal of Computational Chemistry, 2009, 30, 589-600.	3.3	61
21	Electrostatic potential maps of damaged DNA studied by image analysis tools. 8-Oxoguanine and abasic site lesions. Journal of Molecular Modeling, 2009, 15, 817-827.	1.8	2
22	Thermodynamic and Structural Investigations of Ammonium Borohydride, a Solid with a Highest Content of Thermodynamically and Kinetically Accessible Hydrogen. Chemistry of Materials, 2009, 21, 4356-4358.	6.7	55
23	Structure and singly occupied molecular orbital analysis of anionic tautomers of guanine. Journal of Computational Chemistry, 2008, 29, 1277-1291.	3.3	2
24	Visualization of Molecular Orbitals and the Related Electron Densities. Journal of Chemical Theory and Computation, 2008, 4, 689-693.	5.3	30
25	Solvation free energies of molecules. The most stable anionic tautomers of uracil. Physical Chemistry Chemical Physics, 2008, 10, 4442.	2.8	17
26	Cylindrical Projection of Electrostatic Potential and Image Analysis Tools for Damaged DNA:â€‰ The Substitution of Thymine with Thymine Glycol. Journal of Physical Chemistry B, 2008, 112, 2198-2206.	2.6	4
27	Stable Valence Anions of Nucleic Acid Bases and DNA Strand Breaks Induced by Low Energy Electrons. Challenges and Advances in Computational Chemistry and Physics, 2008, , 619-667.	0.6	15
28	Effect of excess electron and one water molecule on relative stability of the canonical and zwitterionic tautomers of glycine. Journal of Chemical Physics, 2008, 128, 125101.	3.0	8
29	Photoelectron spectrum of valence anions of uracil and first-principles calculations of excess electron binding energies. Journal of Chemical Physics, 2008, 129, 054309.	3.0	40
30	Electron-Driven Acid-Base Chemistry: Proton Transfer from Hydrogen Chloride to Ammonia. Science, 2008, 319, 936-939.	12.6	73
31	Coupled-cluster and explicitly correlated perturbation-theory calculations of the uracil anion. Journal of Chemical Physics, 2007, 126, 085101.	3.0	63
32	Photoelectron spectroscopy of adiabatically bound valence anions of rare tautomers of the nucleic acid bases. Journal of Chemical Physics, 2007, 127, 174309.	3.0	59
33	Band offset and magnetic property engineering for epitaxial interfaces: A monolayer ofM2O3(M=Al,Ga,Sc,Ti,Ni)at theÎ±â^'Fe2O3â^•Î±â^'Cr2O3(0001) interface. Physical Review B, 2007, 75, .	3.2	6
34	Bound anionic states of adenine. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 4804-4807.	7.1	60
35	Adiabatically Bound Valence Anions of Guanine. Journal of Physical Chemistry B, 2007, 111, 14073-14076.	2.6	27
36	Valence Anions in Complexes of Adenine and 9-Methyladenine with Formic Acid:Â Stabilization by Intermolecular Proton Transfer. Journal of the American Chemical Society, 2007, 129, 1216-1224.	13.7	37

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37	Isomers and Conformers of H(NH2BH2)nH Oligomers:â€‰ Understanding the Geometries and Electronic Structure of Boronâ^'Nitrogenâ^'Hydrogen Compounds as Potential Hydrogen Storage Materials. Journal of Physical Chemistry C, 2007, 111, 3294-3299.	3.1	38
38	Quantum Mechanical Energy-Based Screening of Combinatorially Generated Library of Tautomers. TauTGen:â€‰ A Tautomer Generator Program. Journal of Chemical Information and Modeling, 2007, 47, 686-694.	5.4	34
39	Driving force for the WO3(001) surface relaxation. Surface Science, 2007, 601, 1481-1488.	1.9	40
40	Intermolecular proton transfer induced by excess electron attachment to adenine(formic acid)n (n=2,) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.9	20
41	Differences in electrostatic potential around DNA fragments containing adenine and 8-oxo-adenine. Journal of Molecular Graphics and Modelling, 2007, 26, 282-289.	2.4	6
42	Can an excess electron localize on a purine moiety in the adenine-thymine Watson-Crick base pair? A computational study. International Journal of Quantum Chemistry, 2007, 107, 2224-2232.	2.0	8
43	Differences in electrostatic potential around DNA fragments containing guanine and 8-oxo-guanine. Theoretical Chemistry Accounts, 2007, 117, 291-296.	1.4	4
44	Gaseous Arginine Conformers and Their Unique Intramolecular Interactions. Journal of Physical Chemistry A, 2006, 110, 12282-12291.	2.5	100
45	On the Unusual Stability of Valence Anions of Thymine Based on Very Rare Tautomers:Â A Computational Study. Journal of Physical Chemistry B, 2006, 110, 24696-24707.	2.6	44
46	DNA strand breaks induced by concerted interaction of H radicals and low-energy electrons. European Physical Journal D, 2005, 35, 429-435.	1.3	64
47	Nanoscaffold Mediates Hydrogen Release and the Reactivity of Ammonia Borane. Angewandte Chemie - International Edition, 2005, 44, 3578-3582.	13.8	751
48	Finding Adiabatically Bound Anions of Guanine through a Combinatorial Computational Approach. Angewandte Chemie - International Edition, 2005, 44, 6585-6588.	13.8	43
49	Thermodynamic Properties of Molecular Borane Amines and the [BH4-][NH4+] Salt for Chemical Hydrogen Storage Systems from ab initio Electronic Structure Theory.. ChemInform, 2005, 36, no.	0.0	0
50	Intermolecular Proton Transfer in Anionic Complexes of Uracil with Alcohols. Journal of Physical Chemistry B, 2005, 109, 13383-13391.	2.6	55
51	Structure and Energetics of Clustered Damage Sites. Radiation Research, 2005, 164, 582-585.	1.5	4
52	Stabilization of very rare tautomers of uracil by an excess electron. Physical Chemistry Chemical Physics, 2005, 7, 2116.	2.8	73
53	Electronic Structure Differences in ZrO2vs HfO2â€. Journal of Physical Chemistry A, 2005, 109, 11521-11525.	2.5	114
54	Valence and Dipole-Bound Anions of the Most Stable Tautomers of Guanine. Journal of the American Chemical Society, 2005, 127, 699-706.	13.7	84

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55	Low-temperature polymorphs ofZrO2andHfO2: A density-functional theory study. Physical Review B, 2005, 72, .	3.2	194
56	AT Base Pair Anions versus (9-Methyl-A)(1-Methyl-T) Base Pair Anions. Journal of the American Chemical Society, 2005, 127, 6443-6450.	13.7	84
57	Stabilization of Very Rare Tautomers of 1-Methylcytosine by an Excess Electronâ€. Journal of Physical Chemistry A, 2005, 109, 11495-11503.	2.5	32
58	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€‰ Issues and Scientific Advances. Chemical Reviews, 2005, 105, 355-390.	47.7	560
59	Thermodynamic Properties of Molecular Borane Amines and the [BH4-][NH4+] Salt for Chemical Hydrogen Storage Systems from ab Initio Electronic Structure Theory. Journal of Physical Chemistry A, 2005, 109, 5129-5135.	2.5	198
60	Anion of the formic acid dimer as a model for intermolecular proton transfer induced by a Ï€* excess electron. Journal of Chemical Physics, 2005, 122, 204304.	3.0	23
61	Interaction with Glycine Increases Stability of a Mutagenic Tautomer of Uracil. A Density Functional Theory Study. Journal of the American Chemical Society, 2005, 127, 2238-2248.	13.7	34
62	Barrier-free intermolecular proton transfer induced by excess electron attachment to the complex of alanine with uracil. Journal of Chemical Physics, 2004, 120, 6064-6071.	3.0	55
63	First-principles study of noncommutative band offsets atÎ±â^'Cr2O3/Î±â^'Fe2O3(0001)interfaces. Physical Review B, 2004, 69, .	3.2	32
64	SrTiO3â^•Si(001)epitaxial interface: A density functional theory study. Physical Review B, 2004, 70, .	3.2	32
65	Accurate valence band maximum determination for SrTiO3(001). Surface Science, 2004, 554, 81-89.	1.9	78
66	Barrier-free proton transfer in anionic complex of thymine with glycine. Physical Chemistry Chemical Physics, 2004, 6, 4351-4357.	2.8	49
67	Experimental determination of valence band maxima for SrTiO[sub 3], TiO[sub 2], and SrO and the associated valence band offsets with Si(001). Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2004, 22, 2205.	1.6	251
68	Excess Electron Attachment Induces Barrier-Free Proton Transfer in Anionic Complexes of Thymine and Uracil with Formic Acid. Journal of Physical Chemistry B, 2004, 108, 6919-6921.	2.6	44
69	Effect of Hydrogen Bonding on Barrier-Free Proton Transfer in Anionic Complexes of Uracil with Weak Acids: (Uâ€¦HCN)â^versus (Uâ€¦H2S)â^'. Israel Journal of Chemistry, 2004, 44, 157-170.	2.3	28
70	Structural Criteria for the Rational Design of Selective Ligands:â€‰ Convergent Hydrogen Bonding Sites for the Nitrate Anion. Journal of the American Chemical Society, 2004, 126, 7925-7934.	13.7	89
71	Consequences of Proton Transfer in Guanidine. ChemInform, 2003, 34, no.	0.0	0
72	Consequences of proton transfer in guanidine. Journal of Physical Organic Chemistry, 2003, 16, 91-106.	1.9	109

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73	Excess Electron Attachment Induces Barrier-Free Proton Transfer in Binary Complexes of Uracil with H2Se and H2S but Not with H2O. Journal of Physical Chemistry B, 2003, 107, 7889-7895.	2.6	53
74	Formation of thec(1Ã—1)Cu monolayer on CaO(100):â€ƒA theoretical study. Physical Review B, 2003, 68, .	3.2	6
75	Solvated Electrons in Very Small Clusters of Polar Molecules:(HF)3â¯. Physical Review Letters, 2002, 88, 143001.	7.8	62
76	Electron binding energies of dipole-bound anions at the coupled cluster level with single, double, and triple excitations: HCNâ¯ and HNCâ¯. Journal of Chemical Physics, 2002, 116, 3297-3299.	3.0	27
77	Oxides, Silicides, and Silicates of Zirconium and Hafnium; Density Functional Theory Study. Materials Research Society Symposia Proceedings, 2002, 716, 651.	0.1	0
78	Computational Study of Hydrogen-Bonded Complexes between the Most Stable Tautomers of Glycine and Uracil. Journal of Physical Chemistry A, 2002, 106, 7423-7433.	2.5	49
79	Thermodynamic stability of high-K dielectric metal oxides ZrO2 and HfO2 in contact with Si and SiO2. Applied Physics Letters, 2002, 80, 1897-1899.	3.3	346
80	Barrier-free intermolecular proton transfer in the uracil-glycine complex induced by excess electron attachment. European Physical Journal D, 2002, 20, 431-439.	1.3	73
81	Low-Energy Tautomers and Conformers of Neutral and Protonated Arginine. Journal of the American Chemical Society, 2001, 123, 11695-11707.	13.7	133
82	Photoinduced nonadiabatic dynamics in quartet Na[sub 3] and K[sub 3] formed using helium nanodroplet isolation. Journal of Chemical Physics, 2001, 115, 10265.	3.0	51
83	Quasidegeneracy of Zwitterionic and Canonical Tautomers of Arginine Solvated by an Excess Electron. Journal of the American Chemical Society, 2001, 123, 11073-11074.	13.7	64
84	Anab initiostudy of the betaine anionâ€“dipole-bound anionic state of a model zwitterion system. Journal of Chemical Physics, 2001, 114, 10673-10681.	3.0	49
85	Non-ionic and zwitterionic forms of neutral arginine â€“ an ab initio study. Chemical Physics Letters, 2001, 337, 143-150.	2.6	50
86	Ab initio electronic structure of HCNâ¯ and HNCâ¯ dipole-bound anions and a description of electron loss upon tautomerization. Journal of Chemical Physics, 2001, 114, 7443-7449.	3.0	32
87	On the possibility of binding of two electrons to dipole potentials. International Journal of Quantum Chemistry, 2000, 76, 197-204.	2.0	15
88	How to choose a one-electron basis set to reliably describe a dipole-bound anion. International Journal of Quantum Chemistry, 2000, 80, 1024-1038.	2.0	141
89	A bi-dipole-bound dianion. Chemical Physics Letters, 2000, 322, 175-180.	2.6	12
90	Bi-dipole-bound anions. International Journal of Mass Spectrometry, 2000, 201, 245-252.	1.5	11

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91	Excited electronic states of the anion of 7,7,8,8-tetracyanoquinodimethane (TCNQ). Computational and Theoretical Chemistry, 2000, 531, 339-348.	1.5	21
92	Opposite rumpling of the MgO and CaO (100) surfaces: A density-functional theory study. Physical Review B, 2000, 62, 8318-8322.	3.2	38
93	Anab initiostudy of (H3Bâ†NH3)â^'â€"a dipole-bound anion supported by the dative charge-transfer bond in the neutral host. Journal of Chemical Physics, 2000, 113, 8961-8968.	3.0	14
94	(MgO)nâ^'(n=1â€"5)Clusters: Multipole-Bound Anions and Photodetachment Spectroscopy. Physical Review Letters, 2000, 85, 3145-3148.	7.8	51
95	LDA and GGA calculations of alkali metal adsorption at the (001) surface of MgO. Journal of Chemical Physics, 2000, 112, 3014-3022.	3.0	38
96	Comparison of embedded-atom models and first-principles calculations for Al phase equilibrium. Computational Materials Science, 2000, 18, 199-204.	3.0	9
97	First-principles studies of adsorption of CO on the Na(100) surface. Surface Science, 2000, 453, 130-136.	1.9	4
98	High-coverage adsorption of alkali metals at the CaO and MgO (100) surfaces. Surface Science, 2000, 466, 111-118.	1.9	16
99	Adsorption of CO on MgO supported alkali monolayers: a periodic density functional local density approximation and generalized gradient approximation study. Surface Science, 2000, 445, 495-505.	1.9	18
100	Periodic Density Functional LDA and GGA Study of CO Adsorption at the (001) Surface of MgO. Journal of Physical Chemistry B, 2000, 104, 4717-4722.	2.6	37
101	Dipole-Bound Anions of Glycine Based on the Zwitterion and Neutral Structures. Journal of the American Chemical Society, 2000, 122, 10159-10162.	13.7	133
102	On the importance of exchange effects in three-body interactions: The lowest quartet state of Na3. Journal of Chemical Physics, 2000, 112, 5751-5761.	3.0	61
103	How to choose a oneâ€electron basis set to reliably describe a dipoleâ€bound anion. International Journal of Quantum Chemistry, 2000, 80, 1024-1038.	2.0	4
104	Mixed valence/dipole-bound dianions. Journal of Chemical Physics, 1999, 111, 9469-9474.	3.0	16
105	Theoretical study of the dipole-bound anion (HPPH3)â^'. Journal of Chemical Physics, 1999, 110, 274-280.	3.0	40
106	Highly accurate ab initio calculation of the interaction potential for two sodium atoms with parallel spins. Journal of Chemical Physics, 1999, 110, 4695-4698.	3.0	20
107	Electron binding energies in linear dipole-bound (HCN)nâ^' (n=2â€"5) anions. Chemical Physics Letters, 1999, 300, 331-338.	2.6	23
108	Theoretical study of the quadrupole-bound anion (BeO)2â^'. Chemical Physics Letters, 1999, 303, 65-75.	2.6	23

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109	Favorable performance of the DFT methods in predicting the minimum-energy structure of the lowest triplet state of WF4. International Journal of Quantum Chemistry, 1999, 73, 369-375.	2.0	2
110	Ab initio study of the dipole-bound anion (H2Oâ€¦HCl)â^'. Journal of Chemical Physics, 1999, 111, 3004-3011.	3.0	7
111	Dipole-Bound Anion of the HNNH3Isomer of Hydrazine. An Ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 625-631.	2.5	31
112	Helium Cluster Isolation Spectroscopy of Alkali Dimers in the Triplet Manifold. Journal of Physical Chemistry A, 1998, 102, 4952-4965.	2.5	149
113	Electronic Structure of Dipole-Bound Anions. Journal of Physical Chemistry A, 1998, 102, 2624-2633.	2.5	148
114	Theoretical study of the dipole-bound anion (H2Oâ€¦NH3)â^'. Journal of Chemical Physics, 1998, 108, 6303-6311.	3.0	44
115	Theoretical study of the dipole-bound anion (HF)2â^'. Journal of Chemical Physics, 1997, 107, 2968-2973.	3.0	56
116	Dispersion Stabilization of Solvated Electrons and Dipole-Bound Anions. Journal of Physical Chemistry B, 1997, 101, 9143-9146.	2.6	88
117	Hartreeâ^'Fock and Density Functional Methods and IR and NMR Spectroscopies in the Examination of Tautomerism and Features of Neutral 9-Acridinamine in Gaseous and Condensed Media. Journal of Physical Chemistry A, 1997, 101, 283-292.	2.5	39
118	Energies of dipole-bound anionic states. International Journal of Quantum Chemistry, 1997, 64, 183-191.	2.0	86
119	Small Multiply Charged Anions as Building Blocks in Chemistry. Accounts of Chemical Research, 1996, 29, 497-502.	15.6	170
120	Properties of Closed-Shell, Octahedral, Multiply-Charged Hexafluorometallates MF63-, M = Sc, Y, La, ZrF62-, and TaF6-. Journal of the American Chemical Society, 1996, 118, 1173-1180.	13.7	59
121	Photoinduced Chemical Dynamics of High-Spin Alkali Trimers. Science, 1996, 273, 629-631.	12.6	157
122	Spin Polarized Alkali Clusters: Observation of Quartet States of the Sodium Trimer. Physical Review Letters, 1996, 77, 4532-4535.	7.8	90
123	Contribution of electron correlation to the stability of dipole-bound anionic states. Physical Review A, 1996, 54, 1906-1909.	2.5	167
124	Autodetachment spectroscopy and dynamics of vibrationally excited dipoleâ€bound states of H2CCCâ^'. Journal of Chemical Physics, 1996, 105, 10706-10718.	3.0	84
125	Comment on â€œA possible definition of basis set superposition errorâ€• Chemical Physics Letters, 1995, 241, 140-145.	2.6	23
126	On the possibilities of theoretical analysis of kinetics of the thermal decomposition of solids. Journal of Thermal Analysis, 1995, 43, 45-55.	0.6	9

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127	Thermodynamics of the thermal decomposition of calcium oxalate monohydrate examined theoretically. Journal of Thermal Analysis, 1995, 43, 239-246.	0.6	18
128	Anionic and Neutral States of Li3O. The Journal of Physical Chemistry, 1994, 98, 8326-8330.	2.9	31
129	Theoretical Studies on the Geometry, Thermochemistry, Vibrational Spectroscopy, and Charge Distribution in TiX62- (X = F, Cl, Br, I). Coulombic Energy in hexahalogenotitanate Lattices. The Journal of Physical Chemistry, 1994, 98, 6280-6286.	2.9	8
130	Theoretical studies on structure, thermochemistry, vibrational spectroscopy, and other features of ZrX2â^'6(X=F,Cl,Br,I): Coulombic energy in inorganic and organic hexahalogenozirconates. Journal of Chemical Physics, 1994, 100, 5810-5820.	3.0	18
131	Ab initiostudy of He(1S)+Cl2(Xâ€‰1Î£g,3Îu) potential energy surfaces. Journal of Chemical Physics, 1994, 101, 6800-6809.	3.0	36
132	New anionic states of the lithium trimer. Journal of Chemical Physics, 1994, 101, 4867-4877.	3.0	13
133	Anionic states of LiFLi. Journal of Chemical Physics, 1994, 100, 1308-1311.	3.0	28
134	Potential energy curves of M(npâ€‰2P)â‹…RG(2Î) excited states and M+â‹…RG ground states (M=Li, Na; RG=He, Ne). Journal of Chemical Physics, 1994, 100, 8212-8218.	3.0	38
135	Vertical Electron Detachment Energies for Octahedral Closed-Shell Multiply-Charged Anions. Journal of the American Chemical Society, 1994, 116, 9262-9268.	13.7	47
136	Theoretical Studies on the Structure, Thermochemistry, Vibrational Spectroscopy, and Other Features of HfX62- (X = F, Cl, Br, I). Electrostatic Energy in Hexahalogenohafnates. Inorganic Chemistry, 1994, 33, 6187-6193.	4.0	13
137	Critical evaluation of some computational approaches to the problem of basis set superposition error. Journal of Chemical Physics, 1993, 98, 5540-5554.	3.0	143
138	Accuracy of the Boys and Bernardi function counterpoise method. Journal of Chemical Physics, 1993, 98, 4728-4737.	3.0	212
139	Singletâ€toâ€triplet energy transfer via 1Î1/3Î£+1 curve crossings in group 2 and 12 metalâ€“atom/rareâ€gas systems. Journal of Chemical Physics, 1993, 99, 3815-3822.	3.0	14
140	Collisional energy transfer in bimolecular ionâ€“molecule dynamics M++(H2; D2; or HD)â†'(MH++H;) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	3.0	11
141	Reaction potential surface for boron(1+)(1S) + hydrogen .fwdarw. HBH+(1.SIGMA.g+), BH+(2.SIGMA.) + hydrogen atom (2S). The Journal of Physical Chemistry, 1992, 96, 644-650.	2.9	19
142	Ab initio potentialâ€energy surfaces for Cd(1P)+H2=CdH(Xâ€‰2Î£+)+H, HCdH(Xâ€‰1Î£+g), Cd(3P)+H2, and Cd(1S)+H+H. Journal of Chemical Physics, 1992, 96, 6555-6564.	3.0	18
143	Relative stabilities of fullerene, cumulene, and polyacetylene structures for Cnâ€‰:n=18â€“60. Journal of Chemical Physics, 1992, 96, 2926-2932.	3.0	160
144	Self-Consistent-Field potential-energy surfaces for hydrogen atom pairs within small palladium clusters. International Journal of Quantum Chemistry, 1992, 41, 793-810.	2.0	3

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145	Double-Rydberg molecular anions. Chemical Reviews, 1991, 91, 669-677.	47.7	47
146	Ab initio quantum chemistry study of formamide-formamidic acid tautomerization. The Journal of Physical Chemistry, 1991, 95, 10419-10424.	2.9	107
147	Interpretation of the hydrogen-bond energy at the Hartree-Fock level for pairs of the hydrogen fluoride, water and ammonia molecules. The Journal of Physical Chemistry, 1990, 94, 5710-5714.	2.9	14
148	Doubleâ€Rydberg anions: Groundâ€state electronic and geometric stabilities. Journal of Chemical Physics, 1990, 93, 3874-3880.	3.0	74
149	Lifetimes of electronically metastable doubleâ€Rydberg anions: FHâ^'2. Journal of Chemical Physics, 1990, 93, 2546-2553.	3.0	9
150	The Ab initio energy and structure of hydride-hydrogen (H-(H2)2). The Journal of Physical Chemistry, 1989, 93, 621-625.	2.9	18
151	Weak interactions between small systems. Models for studying the nature of intermolecular forces and challenging problems for ab initio calculations. Chemical Reviews, 1988, 88, 943-962.	47.7	266
152	"Dougle-Rydberg" molecular anions. The Journal of Physical Chemistry, 1988, 92, 6179-6182.	2.9	29
153	Interpretation of the Hartree-Fock interaction energy between closed-shell systems. Molecular Physics, 1988, 64, 337-355.	1.7	99
154	Proper correction for the basis set superposition error in SCF calculations of intermolecular interactions. Molecular Physics, 1987, 61, 233-247.	1.7	138
155	The impact of higher polarization functions of second-order dispersion energy. Partial wave expansion and damping phenomenon for He2. Chemical Physics, 1987, 111, 271-283.	1.9	93
156	Does the boys and bernardi function counterpoise method actually overcorrect the basis set superposition error?. Chemical Physics Letters, 1986, 129, 325-328.	2.6	75
157	The basis set superposition error in correlated electronic structure calculations. Chemical Physics Letters, 1986, 124, 370-375.	2.6	212
158	Dimer centred basis set in the calculations of the first-order interaction energy with CI wavefunction. Molecular Physics, 1985, 54, 1173-1184.	1.7	39
159	Effective basis sets for calculations of exchange-repulsion energy. International Journal of Quantum Chemistry, 1984, 26, 971-982.	2.0	69
160	Importance of exchange effects in the deformation of interacting ions. International Journal of Quantum Chemistry, 1983, 23, 1843-1853.	2.0	21
161	Approximate exchange and electrostatic interaction energies of deformed ions. International Journal of Quantum Chemistry, 1981, 19, 401-411.	2.0	3