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	Nanoscaffold Mediates Hydrogen Release and the Reactivity of Ammonia Borane. Angewandte Chemie - International Edition, 2005, 44, 3578-3582.	13.8	751
2	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€‰ Issues and Scientific Advances. Chemical Reviews, 2005, 105, 355-390.	47.7	560
3	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
4	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
5	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
6	The basis set superposition error in correlated electronic structure calculations. Chemical Physics Letters, 1986, 124, 370-375.	2.6	212
7	Accuracy of the Boys and Bernardi function counterpoise method. Journal of Chemical Physics, 1993, 98, 4728-4737.	3.0	212
8	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
9	Low-temperature polymorphs ofZrO2andHfO2: A density-functional theory study. Physical Review B, 2005, 72, .	3.2	194
10	Small Multiply Charged Anions as Building Blocks in Chemistry. Accounts of Chemical Research, 1996, 29, 497-502.	15.6	170
11	Contribution of electron correlation to the stability of dipole-bound anionic states. Physical Review A, 1996, 54, 1906-1909.	2.5	167
12	Relative stabilities of fullerene, cumulene, and polyacetylene structures for Cnâ€‰:n=18â€“60. Journal of Chemical Physics, 1992, 96, 2926-2932.	3.0	160
13	Photoinduced Chemical Dynamics of High-Spin Alkali Trimers. Science, 1996, 273, 629-631.	12.6	157
14	Helium Cluster Isolation Spectroscopy of Alkali Dimers in the Triplet Manifold. Journal of Physical Chemistry A, 1998, 102, 4952-4965.	2.5	149
15	Electronic Structure of Dipole-Bound Anions. Journal of Physical Chemistry A, 1998, 102, 2624-2633.	2.5	148
16	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
17	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
18	Proper correction for the basis set superposition error in SCF calculations of intermolecular interactions. Molecular Physics, 1987, 61, 233-247.	1.7	138

#	Article	IF	Citations
19	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
20	Low-Energy Tautomers and Conformers of Neutral and Protonated Arginine. Journal of the American Chemical Society, 2001, 123, 11695-11707.	13.7	133
21	Electronic Structure Differences in ZrO2vs HfO2â€. Journal of Physical Chemistry A, 2005, 109, 11521-11525.	2.5	114
22	Consequences of proton transfer in guanidine. Journal of Physical Organic Chemistry, 2003, 16, 91-106.	1.9	109
23	Ab initio quantum chemistry study of formamide-formamidic acid tautomerization. The Journal of Physical Chemistry, 1991, 95, 10419-10424.	2.9	107
24	Gaseous Arginine Conformers and Their Unique Intramolecular Interactions. Journal of Physical Chemistry A, 2006, 110, 12282-12291.	2.5	100
25	Interpretation of the Hartree-Fock interaction energy between closed-shell systems. Molecular Physics, 1988, 64, 337-355.	1.7	99
26	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
27	Spin Polarized Alkali Clusters: Observation of Quartet States of the Sodium Trimer. Physical Review Letters, 1996, 77, 4532-4535.	7.8	90
28	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
29	Dispersion Stabilization of Solvated Electrons and Dipole-Bound Anions. Journal of Physical Chemistry B, 1997, 101, 9143-9146.	2.6	88
30	Energies of dipole-bound anionic states. International Journal of Quantum Chemistry, 1997, 64, 183-191.	2.0	86
31	Autodetachment spectroscopy and dynamics of vibrationally excited dipoleâ€bound states of H2CCCâ¯. Journal of Chemical Physics, 1996, 105, 10706-10718.	3.0	84
32	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
33	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
34	Accurate valence band maximum determination for SrTiO3(001). Surface Science, 2004, 554, 81-89.	1.9	78
35	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
36	Doubleâ€Rydberg anions: Groundâ€state electronic and geometric stabilities. Journal of Chemical Physics, 1990, 93, 3874-3880.	3.0	74

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37	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
38	Stabilization of very rare tautomers of uracil by an excess electron. Physical Chemistry Chemical Physics, 2005, 7, 2116.	2.8	73
39	Electron-Driven Acid-Base Chemistry: Proton Transfer from Hydrogen Chloride to Ammonia. Science, 2008, 319, 936-939.	12.6	73
40	Effective basis sets for calculations of exchange-repulsion energy. International Journal of Quantum Chemistry, 1984, 26, 971-982.	2.0	69
41	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
42	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
43	Coupled-cluster and explicitly correlated perturbation-theory calculations of the uracil anion. Journal of Chemical Physics, 2007, 126, 085101.	3.0	63
44	Solvated Electrons in Very Small Clusters of Polar Molecules:(HF)3â¯. Physical Review Letters, 2002, 88, 143001.	7.8	62
45	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
46	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
47	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
48	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
49	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
50	Theoretical study of the dipole-bound anion (HF)2â¯. Journal of Chemical Physics, 1997, 107, 2968-2973.	3.0	56
51	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
52	Intermolecular Proton Transfer in Anionic Complexes of Uracil with Alcohols. Journal of Physical Chemistry B, 2005, 109, 13383-13391.	2.6	55
53	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
54	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

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55	(MgO)nâ^'(n=1â€“5)Clusters: Multipole-Bound Anions and Photodetachment Spectroscopy. Physical Review Letters, 2000, 85, 3145-3148.	7.8	51
56	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
57	Non-ionic and zwitterionic forms of neutral arginine â€“ an ab initio study. Chemical Physics Letters, 2001, 337, 143-150.	2.6	50
58	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
59	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
60	Barrier-free proton transfer in anionic complex of thymine with glycine. Physical Chemistry Chemical Physics, 2004, 6, 4351-4357.	2.8	49
61	Double-Rydberg molecular anions. Chemical Reviews, 1991, 91, 669-677.	47.7	47
62	Vertical Electron Detachment Energies for Octahedral Closed-Shell Multiply-Charged Anions. Journal of the American Chemical Society, 1994, 116, 9262-9268.	13.7	47
63	Theoretical study of the dipole-bound anion (H2Oâ€¦NH3)â^'. Journal of Chemical Physics, 1998, 108, 6303-6311.	3.0	44
64	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
65	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
66	Finding Adiabatically Bound Anions of Guanine through a Combinatorial Computational Approach. Angewandte Chemie - International Edition, 2005, 44, 6585-6588.	13.8	43
67	Theoretical study of the dipole-bound anion (HPPH3)â^'. Journal of Chemical Physics, 1999, 110, 274-280.	3.0	40
68	Driving force for the WO3(001) surface relaxation. Surface Science, 2007, 601, 1481-1488.	1.9	40
69	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
70	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
71	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
72	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

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73	Opposite rumpling of the MgO and CaO (100) surfaces: A density-functional theory study. Physical Review B, 2000, 62, 8318-8322.	3.2	38
74	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
75	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
76	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
77	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
78	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
79	Ab initiostudy of He(1S)+Cl2(Xâ€‰1Î£g,3Îu) potential energy surfaces. Journal of Chemical Physics, 1994, 101, 6800-6809.	3.0	36
80	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
81	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
82	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
83	First-principles study of noncommutative band offsets atÎ±â^'Cr2O3/Î±â^'Fe2O3(0001)interfaces. Physical Review B, 2004, 69, .	3.2	32
84	SrTiO3â^•Si(001)epitaxial interface: A density functional theory study. Physical Review B, 2004, 70, .	3.2	32
85	Stabilization of Very Rare Tautomers of 1-Methylcytosine by an Excess Electronâ€. Journal of Physical Chemistry A, 2005, 109, 11495-11503.	2.5	32
86	Anionic and Neutral States of Li3O. The Journal of Physical Chemistry, 1994, 98, 8326-8330.	2.9	31
87	Dipole-Bound Anion of the HNNH3Isomer of Hydrazine. An Ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 625-631.	2.5	31
88	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
89	Visualization of Molecular Orbitals and the Related Electron Densities. Journal of Chemical Theory and Computation, 2008, 4, 689-693.	5.3	30
90	"Dougle-Rydberg" molecular anions. The Journal of Physical Chemistry, 1988, 92, 6179-6182.	2.9	29

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91	Anionic states of LiFLi. Journal of Chemical Physics, 1994, 100, 1308-1311.	3.0	28
92	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
93	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
94	Adiabatically Bound Valence Anions of Guanine. Journal of Physical Chemistry B, 2007, 111, 14073-14076.	2.6	27
95	Comment on â€œA possible definition of basis set superposition errorâ€• Chemical Physics Letters, 1995, 241, 140-145.	2.6	23
96	Electron binding energies in linear dipole-bound (HCN)nâ^ (n=2â€“5) anions. Chemical Physics Letters, 1999, 300, 331-338.	2.6	23
97	Theoretical study of the quadrupole-bound anion (BeO)2â^. Chemical Physics Letters, 1999, 303, 65-75.	2.6	23
98	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
99	Importance of exchange effects in the deformation of interacting ions. International Journal of Quantum Chemistry, 1983, 23, 1843-1853.	2.0	21
100	Excited electronic states of the anion of 7,7,8,8-tetracyanoquinodimethane (TCNQ). Computational and Theoretical Chemistry, 2000, 531, 339-348.	1.5	21
101	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
102	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
103	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
104	The Ab initio energy and structure of hydride-hydrogen (H-(H2)2). The Journal of Physical Chemistry, 1989, 93, 621-625.	2.9	18
105	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
106	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
107	Thermodynamics of the thermal decomposition of calcium oxalate monohydrate examined theoretically. Journal of Thermal Analysis, 1995, 43, 239-246.	0.6	18
108	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

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109	Solvation free energies of molecules. The most stable anionic tautomers of uracil. Physical Chemistry Chemical Physics, 2008, 10, 4442.	2.8	17
110	Mixed valence/dipole-bound dianions. Journal of Chemical Physics, 1999, 111, 9469-9474.	3.0	16
111	High-coverage adsorption of alkali metals at the CaO and MgO (100) surfaces. Surface Science, 2000, 466, 111-118.	1.9	16
112	Is Electronegativity a Useful Descriptor for the Pseudoâ€Alkali Metal NH₄?. Chemistry - A European Journal, 2011, 17, 13197-13205.	3.3	16
113	On the possibility of binding of two electrons to dipole potentials. International Journal of Quantum Chemistry, 2000, 76, 197-204.	2.0	15
114	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
115	Ammoniaâˆ'Hydrogen Bromide and Ammoniaâˆ'Hydrogen Iodide Complexes: Anion Photoelectron and ab Initio Studies. Journal of Physical Chemistry A, 2010, 114, 1357-1363.	2.5	15
116	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
117	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
118	Anab initiostudy of (H3Bâ†NH3)âˆ'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
119	New anionic states of the lithium trimer. Journal of Chemical Physics, 1994, 101, 4867-4877.	3.0	13
120	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
121	A bi-dipole-bound dianion. Chemical Physics Letters, 2000, 322, 175-180.	2.6	12
122	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
123	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
124	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
125	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
126	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

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127	Bi-dipole-bound anions. International Journal of Mass Spectrometry, 2000, 201, 245-252.	1.5	11
128	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
129	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
130	Lifetimes of electronically metastable doubleâ€Rydberg anions: FHâ^'2. Journal of Chemical Physics, 1990, 93, 2546-2553.	3.0	9
131	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
132	Comparison of embedded-atom models and first-principles calculations for Al phase equilibrium. Computational Materials Science, 2000, 18, 199-204.	3.0	9
133	Non-linear and non-local behaviour in spontaneously electrical solids. Physical Chemistry Chemical Physics, 2018, 20, 5112-5116.	2.8	9
134	Assigning a structural motif using spontaneous molecular dipole orientation in thin films. Physical Chemistry Chemical Physics, 2018, 20, 29038-29044.	2.8	9
135	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
136	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
137	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
138	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
139	Ab initio study of the dipole-bound anion (H2Oâ€¦HCl)â^'. Journal of Chemical Physics, 1999, 111, 3004-3011.	3.0	7
140	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
141	SSC: A tool for constructing libraries for systematic screening of conformers. Journal of Computational Chemistry, 2011, 32, 2047-2054.	3.3	7
142	Formation of thec(1Ã—1)Cu monolayer on CaO(100):â€ƒA theoretical study. Physical Review B, 2003, 68, .	3.2	6
143	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
144	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

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145	A Comparative Study of Methanol Adsorption and Dissociation over WO3(001) and ReO3(001). Topics in Catalysis, 2015, 58, 655-664.	2.8	6
146	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
147	First-principles studies of adsorption of CO on the Na(100) surface. Surface Science, 2000, 453, 130-136.	1.9	4
148	Structure and Energetics of Clustered Damage Sites. Radiation Research, 2005, 164, 582-585.	1.5	4
149	Differences in electrostatic potential around DNA fragments containing guanine and 8-oxo-guanine. Theoretical Chemistry Accounts, 2007, 117, 291-296.	1.4	4
150	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
151	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
152	Approximate exchange and electrostatic interaction energies of deformed ions. International Journal of Quantum Chemistry, 1981, 19, 401-411.	2.0	3
153	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
154	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
155	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
156	Structure and singly occupied molecular orbital analysis of anionic tautomers of guanine. Journal of Computational Chemistry, 2008, 29, 1277-1291.	3.3	2
157	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
158	Structure and Stability of Hydrogen Clathrates of Ammonia Borane. Materials Research Society Symposia Proceedings, 2009, 1216, 1.	0.1	1
159	Oxides, Silicides, and Silicates of Zirconium and Hafnium; Density Functional Theory Study. Materials Research Society Symposia Proceedings, 2002, 716, 651.	0.1	0
160	Consequences of Proton Transfer in Guanidine. ChemInform, 2003, 34, no.	0.0	0
161	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