Maciej Gutowski

List of Publications by Citations

161 papers	8,760 citations	52 h-index	89 g-index
166 ext. papers	9,094 ext. citations	6.3 avg, IF	5.63 L-index

#	Paper	IF	Citations
161	Nanoscaffold mediates hydrogen release and the reactivity of ammonia borane. *Angewandte Chemie - International Edition*, **2005**, 44, 3578-82	16.4	711
160	Role of water in electron-initiated processes and radical chemistry: issues and scientific advances. *Chemical Reviews*, **2005**, 105, 355-90	68.1	469
159	Thermodynamic stability of high-K dielectric metal oxides ZrO2 and HfO2 in contact with Si and SiO2. *Applied Physics Letters*, **2002**, 80, 1897-1899	3.4	316
158	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	68.1	252
157	Experimental determination of valence band maxima for SrTiO3, TiO2, 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		240
156	The basis set superposition error in correlated electronic structure calculations. *Chemical Physics Letters*, **1986**, 124, 370-375	2.5	196
155	Accuracy of the Boys and Bernardi function counterpoise method. *Journal of Chemical Physics*, **1993**, 98, 4728-4737	3.9	195
154	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, 5129-35	2.8	184
153	Low-temperature polymorphs of ZrO2 and HfO2: A density-functional theory study. *Physical Review B*, **2005**, 72,	3.3	163
152	Small Multiply Charged Anions as Building Blocks in Chemistry. *Accounts of Chemical Research*, **1996**, 29, 497-502	24.3	156
151	Contribution of electron correlation to the stability of dipole-bound anionic states. *Physical Review A*, **1996**, 54, 1906-1909	2.6	156
150	Photoinduced Chemical Dynamics of High-Spin Alkali Trimers. *Science*, **1996**, 273, 629-31	33.3	148
149	Relative stabilities of fullerene, cumulene, and polyacetylene structures for Cn : n=18–30. *Journal of Chemical Physics*, **1992**, 96, 2926-2932	3.9	144
148	Electronic Structure of Dipole-Bound Anions. *Journal of Physical Chemistry A*, **1998**, 102, 2624-2633	2.8	140
147	Helium Cluster Isolation Spectroscopy of Alkali Dimers in the Triplet Manifold. *Journal of Physical Chemistry A*, **1998**, 102, 4952-4965	2.8	133
146	Proper correction for the basis set superposition error in SCF calculations of intermolecular interactions. *Molecular Physics*, **1987**, 61, 233-247	1.7	132
145	Dipole-Bound Anions of Glycine Based on the Zwitterion and Neutral Structures. *Journal of the American Chemical Society*, **2000**, 122, 10159-10162	16.4	130

144	Low-energy tautomers and conformers of neutral and protonated arginine. *Journal of the American Chemical Society*, **2001**, 123, 11695-707	16.4	128
143	How to choose a one-electron basis set to reliably describe a dipole-bound anion. *International Journal of Quantum Chemistry*, **2000**, 80, 1024-1038	2.1	127
142	Critical evaluation of some computational approaches to the problem of basis set superposition error. *Journal of Chemical Physics*, **1993**, 98, 5540-5554	3.9	127
141	Ab initio quantum chemistry study of formamide-formamidic acid tautomerization. *The Journal of Physical Chemistry*, **1991**, 95, 10419-10424		104
140	Electronic structure differences in ZrO2 vs HfO2. *Journal of Physical Chemistry A*, **2005**, 109, 11521-5	2.8	102
139	Gaseous arginine conformers and their unique intramolecular interactions. *Journal of Physical Chemistry A*, **2006**, 110, 12282-91	2.8	96
138	Interpretation of the Hartree-Fock interaction energy between closed-shell systems. *Molecular Physics*, **1988**, 64, 337-355	1.7	96
137	Consequences of proton transfer in guanidine. *Journal of Physical Organic Chemistry*, **2003**, 16, 91-106	2.1	95
136	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	2.3	90
135	Dispersion Stabilization of Solvated Electrons and Dipole-Bound Anions. *Journal of Physical Chemistry B*, **1997**, 101, 9143-9146	3.4	83
134	Spin Polarized Alkali Clusters: Observation of Quartet States of the Sodium Trimer. *Physical Review Letters*, **1996**, 77, 4532-4535	7.4	83
133	Energies of dipole-bound anionic states. *International Journal of Quantum Chemistry*, **1997**, 64, 183-191	2.1	82
132	AT base pair anions versus (9-methyl-A)(1-methyl-T) base pair anions. *Journal of the American Chemical Society*, **2005**, 127, 6443-50	16.4	82
131	Valence and dipole-bound anions of the most stable tautomers of guanine. *Journal of the American Chemical Society*, **2005**, 127, 699-706	16.4	80
130	Structural criteria for the rational design of selective ligands: convergent hydrogen bonding sites for the nitrate anion. *Journal of the American Chemical Society*, **2004**, 126, 7925-34	16.4	80
129	Autodetachment spectroscopy and dynamics of vibrationally excited dipole-bound states of H2CCC□*Journal of Chemical Physics*, **1996**, 105, 10706-10718	3.9	74
128	Does the boys and bernardi function counterpoise method actually overcorrect the basis set superposition error?. *Chemical Physics Letters*, **1986**, 129, 325-328	2.5	74
127	Stabilization of very rare tautomers of uracil by an excess electron. *Physical Chemistry Chemical Physics*, **2005**, 7, 2116-25	3.6	72

126	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	72
125	Accurate valence band maximum determination for SrTiO3(001). *Surface Science*, **2004**, 554, 81-89	1.8	71
124	Effective basis sets for calculations of exchange-repulsion energy. *International Journal of Quantum Chemistry*, **1984**, 26, 971-982	2.1	68
123	Electron-driven acid-base chemistry: proton transfer from hydrogen chloride to ammonia. *Science*, **2008**, 319, 936-9	33.3	67
122	Double-Rydberg anions: Ground-state electronic and geometric stabilities. *Journal of Chemical Physics*, **1990**, 93, 3874-3880	3.9	66
121	DNA strand breaks induced by concerted interaction of H radicals and low-energy electrons. *European Physical Journal D*, **2005**, 35, 429-435	1.3	63
120	Solvated electrons in very small clusters of polar molecules: (HF)(3)(-). *Physical Review Letters*, **2002**, 88, 143001	7.4	61
119	Quasidegeneracy of zwitterionic and canonical tautomers of arginine solvated by an excess electron. *Journal of the American Chemical Society*, **2001**, 123, 11073-4	16.4	61
118	Coupled-cluster and explicitly correlated perturbation-theory calculations of the uracil anion. *Journal of Chemical Physics*, **2007**, 126, 085101	3.9	59
117	Bound anionic states of adenine. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 4804-7	11.5	58
116	Intermolecular proton transfer in anionic complexes of uracil with alcohols. *Journal of Physical Chemistry B*, **2005**, 109, 13383-91	3.4	55
115	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	16.4	55
114	Theoretical study of the dipole-bound anion (HF)2 *Journal of Chemical Physics*, **1997**, 107, 2968-2973	3.9	54
113	Photoelectron spectroscopy of adiabatically bound valence anions of rare tautomers of the nucleic acid bases. *Journal of Chemical Physics*, **2007**, 127, 174309	3.9	54
112	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	3.5	53
111	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	3.4	53
110	Barrier-free intermolecular proton transfer induced by excess electron attachment to the complex of alanine with uracil. *Journal of Chemical Physics*, **2004**, 120, 6064-71	3.9	52
109	On the importance of exchange effects in three-body interactions: The lowest quartet state of Na3. *Journal of Chemical Physics*, **2000**, 112, 5751-5761	3.9	52

108	Non-ionic and zwitterionic forms of neutral arginine an ab initio study. *Chemical Physics Letters*, **2001**, 337, 143-150	2.5	49
107	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	9.6	48
106	An ab initio study of the betaine anion dipole-bound anionic state of a model zwitterion system. *Journal of Chemical Physics*, **2001**, 114, 10673-10681	3.9	48
105	Barrier-free proton transfer in anionic complex of thymine with glycine. *Physical Chemistry Chemical Physics*, **2004**, 6, 4351-4357	3.6	47
104	Computational Study of Hydrogen-Bonded Complexes between the Most Stable Tautomers of Glycine and Uracil. *Journal of Physical Chemistry A*, **2002**, 106, 7423-7433	2.8	47
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102	Photoinduced nonadiabatic dynamics in quartet Na3 and K3 formed using helium nanodroplet isolation. *Journal of Chemical Physics*, **2001**, 115, 10265	3.9	47
101	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	3.4	44
100	Vertical Electron Detachment Energies for Octahedral Closed-Shell Multiply-Charged Anions. *Journal of the American Chemical Society*, **1994**, 116, 9262-9268	16.4	42
99	On the unusual stability of valence anions of thymine based on very rare tautomers: A computational study. *Journal of Physical Chemistry B*, **2006**, 110, 24696-707	3.4	41
98	Finding adiabatically bound anions of guanine through a combinatorial computational approach. *Angewandte Chemie - International Edition*, **2005**, 44, 6585-8	16.4	41
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96	Double-Rydberg molecular anions. *Chemical Reviews*, **1991**, 91, 669-677	68.1	40
95	Hartree 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	2.8	38
94	Isomers and Conformers of H(NH2BH2)nH Oligomers: Understanding the Geometries and Electronic Structure of Boron Nitrogen Hydrogen Compounds as Potential Hydrogen Storage Materials. *Journal of Physical Chemistry C*, **2007**, 111, 3294-3299	3.8	38
93	Theoretical study of the dipole-bound anion (HPPH3) *Journal of Chemical Physics*, **1999**, 110, 274-280	3.9	38
92	Dimer centred basis set in the calculations of the first-order interaction energy with CI wavefunction. *Molecular Physics*, **1985**, 54, 1173-1184	1.7	38
91	Photoelectron spectrum of valence anions of uracil and first-principles calculations of excess electron binding energies. *Journal of Chemical Physics*, **2008**, 129, 054309	3.9	37

90	Valence anions in complexes of adenine and 9-methyladenine with formic acid: stabilization by intermolecular proton transfer. *Journal of the American Chemical Society*, **2007**, 129, 1216-24	16.4	37
89	Theoretical investigations on the formation and dehydrogenation reaction pathways of H(NH2BH2)(n)H (n = 1-4) oligomers: importance of dihydrogen interactions. *Inorganic Chemistry*, **2010**, 49, 7710-20	5.1	36
88	LDA and GGA calculations of alkali metal adsorption at the (001) surface of MgO. *Journal of Chemical Physics*, **2000**, 112, 3014-3022	3.9	36
87	Opposite rumpling of the MgO and CaO (100) surfaces: A density-functional theory study. *Physical Review B*, **2000**, 62, 8318-8322	3.3	35
86	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	3.4	34
85	Potential energy curves of M(np 2P)?RG(2)excited states and M+?RG ground states (M=Li, Na; RG=He, Ne). *Journal of Chemical Physics*, **1994**, 100, 8212-8218	3.9	34
84	Driving force for the WO3(0 0 1) surface relaxation. *Surface Science*, **2007**, 601, 1481-1488	1.8	33
83	Interaction with glycine increases stability of a mutagenic tautomer of uracil. A density functional theory study. *Journal of the American Chemical Society*, **2005**, 127, 2238-48	16.4	33
82	Ab initio study of He(1S)+Cl2(X 1g,3u) potential energy surfaces. *Journal of Chemical Physics*, **1994**, 101, 6800-6809	3.9	33
81	Stabilization of very rare tautomers of 1-methylcytosine by an excess electron. *Journal of Physical Chemistry A*, **2005**, 109, 11495-503	2.8	32
80	First-principles study of noncommutative band offsets at Cr2O3/Fe2O3(0001) interfaces. *Physical Review B*, **2004**, 69,	3.3	32
79	Quantum mechanical energy-based screening of combinatorially generated library of tautomers. TauTGen: a tautomer generator program. *Journal of Chemical Information and Modeling*, **2007**, 47, 686-94	6.1	31
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77	Reactivity of hydrogen and methanol on (001) surfaces of WO3, ReO3, WO3/ReO3 and ReO3/WO3. *Catalysis Today*, **2011**, 165, 41-48	5.3	29
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74	Effect of Hydrogen Bonding on Barrier-Free Proton Transfer in Anionic Complexes of Uracil with Weak Acids: (U-HCN) versus (U-H2S) *Israel Journal of Chemistry*, **2004**, 44, 157-170	3.4	28
73	Anionic and Neutral States of Li3O. *The Journal of Physical Chemistry*, **1994**, 98, 8326-8330		28

72	Adiabatically bound valence anions of guanine. *Journal of Physical Chemistry B*, **2007**, 111, 14073-6	3.4	27
71	Electron binding energies of dipole-bound anions at the coupled cluster level with single, double, and triple excitations: HCN and HNC *Journal of Chemical Physics*, **2002**, 116, 3297-3299	3.9	27
70	Anionic states of LiFLi. *Journal of Chemical Physics*, **1994**, 100, 1308-1311	3.9	27
69	"Dougle-Rydberg" molecular anions. *The Journal of Physical Chemistry*, **1988**, 92, 6179-6182		26
68	Visualization of Molecular Orbitals and the Related Electron Densities. *Journal of Chemical Theory and Computation*, **2008**, 4, 689-93	6.4	25
67	Anion of the formic acid dimer as a model for intermolecular proton transfer induced by a pi* excess electron. *Journal of Chemical Physics*, **2005**, 122, 204304	3.9	23
66	Comment on A possible definition of basis set superposition error *Chemical Physics Letters*, **1995**, 241, 140-145	2.5	23
65	Electron binding energies in linear dipole-bound (HCN)n (n=2) anions. *Chemical Physics Letters*, **1999**, 300, 331-338	2.5	21
64	Theoretical study of the quadrupole-bound anion (BeO)2 *Chemical Physics Letters*, **1999**, 303, 65-75	2.5	21
63	Importance of exchange effects in the deformation of interacting ions. *International Journal of Quantum Chemistry*, **1983**, 23, 1843-1853	2.1	21
62	Intermolecular proton transfer induced by excess electron attachment to adenine(formic acid)n (n=2, 3) hydrogen-bonded complexes. *Chemical Physics*, **2007**, 342, 215-222	2.3	20
61	Excited electronic states of the anion of 7,7,8,8-tetracyanoquinodimethane (TCNQ). *Computational and Theoretical Chemistry*, **2000**, 531, 339-348		20
60	Highly accurate ab initio calculation of the interaction potential for two sodium atoms with parallel spins. *Journal of Chemical Physics*, **1999**, 110, 4695-4698	3.9	19
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58	The Ab initio energy and structure of hydride-hydrogen (H-(H2)2). *The Journal of Physical Chemistry*, **1989**, 93, 621-625		18
57	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	1.8	17
56	Theoretical studies on structure, thermochemistry, vibrational spectroscopy, and other features of ZrX2 (X=F,Cl,Br,I): Coulombic energy in inorganic and organic hexahalogenozirconates. *Journal of Chemical Physics*, **1994**, 100, 5810-5820	3.9	17
55	Ab initio potential-energy surfaces for Cd(1P)+H2=CdH(X 2)+H, HCdH(X 1 g), Cd(3P)+H2, and Cd(1S)+H+H. *Journal of Chemical Physics*, **1992**, 96, 6555-6564	3.9	17

54	Solvation free energies of molecules. The most stable anionic tautomers of uracil. *Physical Chemistry Chemical Physics*, **2008**, 10, 4442-8	3.6	16
53	Ammonia-hydrogen bromide and ammonia-hydrogen iodide complexes: anion photoelectron and ab initio studies. *Journal of Physical Chemistry A*, **2010**, 114, 1357-63	2.8	14
52	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	0.7	14
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49	Mixed valence/dipole-bound dianions. *Journal of Chemical Physics*, **1999**, 111, 9469-9474	3.9	14
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47	On the possibility of binding of two electrons to dipole potentials. *International Journal of Quantum Chemistry*, **2000**, 76, 197-204	2.1	13
46	Thermodynamics of the thermal decomposition of calcium oxalate monohydrate examined theoretically. *Journal of Thermal Analysis*, **1995**, 43, 239-246		13
45	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		13
44	Singlet-to-triplet energy transfer via 1Π/3Π1 curve crossings in group 2 and 12 metal⁻tom/rare-gas systems. *Journal of Chemical Physics*, **1993**, 99, 3815-3822	3.9	12
43	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	5.1	12
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41	Communication: Remarkable electrophilicity of the oxalic acid monomer: an anion photoelectron spectroscopy and theoretical study. *Journal of Chemical Physics*, **2014**, 140, 221103	3.9	11
40	Influence of prototropic reactions on the absorption and fluorescence spectra of methyl p-dimethylaminobenzoate and its two ortho derivatives. *Journal of Fluorescence*, **2011**, 21, 1749-62	2.4	10
39	A bi-dipole-bound dianion. *Chemical Physics Letters*, **2000**, 322, 175-180	2.5	10
38	New anionic states of the lithium trimer. *Journal of Chemical Physics*, **1994**, 101, 4867-4877	3.9	10
37	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, 14329-40	16.4	9

36	Combinatorial-computational-chemoinformatics (C3) approach to finding and analyzing low-energy tautomers. *Journal of Computer-Aided Molecular Design*, **2010**, 24, 627-38	4.2	9
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33	Non-linear and non-local behaviour in spontaneously electrical solids. *Physical Chemistry Chemical Physics*, **2018**, 20, 5112-5116	3.6	8
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31	Can an excess electron localize on a purine moiety in the adenine□hymine Watson□rick base pair? A computational study. *International Journal of Quantum Chemistry*, **2007**, 107, 2224-2232	2.1	8
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26	Barrier-free proton transfer induced by electron attachment to the complexes between 1-methylcytosine and formic acid. *Molecular Physics*, **2010**, 108, 2621-2631	1.7	7
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17	Formation of the c(1×1) Cu monolayer on CaO(100): A theoretical study. *Physical Review B*, **2003**, 68,	3.3	5
16	On the possibilities of theoretical analysis of kinetics of the thermal decomposition of solids. *Journal of Thermal Analysis*, **1995**, 43, 45-55		5
15	Differences in electrostatic potential around DNA fragments containing guanine and 8-oxo-guanine. *Theoretical Chemistry Accounts*, **2007**, 117, 291-296	1.9	4
14	Structure and energetics of clustered damage sites. *Radiation Research*, **2005**, 164, 582-5	3.1	4
13	Finding Adiabatically Bound Anions of Guanine through a Combinatorial Computational Approach. *Angewandte Chemie*, **2005**, 117, 6743-6746	3.6	4
12	First-principles studies of adsorption of CO on the Na(100) surface. *Surface Science*, **2000**, 453, 130-136	1.8	4
11	How to choose a one-electron basis set to reliably describe a dipole-bound anion **2000**, 80, 1024		4
10	Electrophilicity of oxalic acid monomer is enhanced in the dimer by intermolecular proton transfer. *Physical Chemistry Chemical Physics*, **2017**, 19, 29760-29766	3.6	3
9	Cylindrical projection of electrostatic potential and image analysis tools for damaged DNA: the substitution of thymine with thymine glycol. *Journal of Physical Chemistry B*, **2008**, 112, 2198-206	3.4	3
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7	Structure and singly occupied molecular orbital analysis of anionic tautomers of guanine. *Journal of Computational Chemistry*, **2008**, 29, 1277-91	3.5	2
6	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	2.1	2
5	Self-Consistent-Field potential-energy surfaces for hydrogen atom pairs within small palladium clusters. *International Journal of Quantum Chemistry*, **1992**, 41, 793-810	2.1	2
4	Structure and Stability of Hydrogen Clathrates of Ammonia Borane. *Materials Research Society Symposia Proceedings*, **2009**, 1216, 1		1
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2	Quantum Chemical Calculation of Possible Forms of Electronic-Vibrational Coupling for FH(CN)⁻ Defects. *Physica Status Solidi A*, **1990**, 117, K115-K118		1
1	Oxides, Silicides, and Silicates of Zirconium and Hafnium; Density Functional Theory Study. *Materials Research Society Symposia Proceedings*, **2002**, 716, 651		