Waclaw Andrzej Sokalski

List of Publications by Citations

109 papers	3,357 citations	31 h-index	54 g-index
117 ext. papers	3,540 ext. citations	3.3 avg, IF	5.1 L-index

#	Paper	IF	Citations
109	Quantitative classification of covalent and noncovalent H-bonds. *Journal of Physical Chemistry B*, **2006**, 110, 6444-6	3.4	197
108	An efficient procedure for decomposition of the SCF interaction energy into components with reduced basis set dependence. *Chemical Physics Letters*, **1988**, 153, 153-159	2.5	187
107	Cumulative atomic multipole representation of the molecular charge distribution and its basis set dependence. *Chemical Physics Letters*, **1983**, 98, 86-92	2.5	187
106	Double-proton transfer in adenine-thymine and guanine-cytosine base pairs. A post-Hartree-Fock ab initio study. *Journal of the American Chemical Society*, **2004**, 126, 10119-29	16.4	185
105	How short can the H...H intermolecular contact be? New findings that reveal the covalent nature of extremely strong interactions. *Journal of Physical Chemistry A*, **2005**, 109, 4331-41	2.8	172
104	Correlated molecular and cumulative atomic multipole moments. *Journal of Chemical Physics*, **1987**, 87, 526-534	3.9	101
103	Transition state stabilization and substrate strain in enzyme catalysis: ab initio QM/MM modelling of the chorismate mutase reaction. *Organic and Biomolecular Chemistry*, **2004**, 2, 968-80	3.9	94
102	Differential transition-state stabilization in enzyme catalysis: quantum chemical analysis of interactions in the chorismate mutase reaction and prediction of the optimal catalytic field. *Journal of the American Chemical Society*, **2004**, 126, 16148-59	16.4	88
101	Nature of X□H+□□□H□ Dihydrogen Bonds and X□H□□□ Interactions. *Journal of Physical Chemistry A*, **2004**, 108, 5823-5830	2.8	87
100	The possible covalent nature of N-H...O hydrogen bonds in formamide dimer and related systems: an ab initio study. *Journal of Physical Chemistry A*, **2006**, 110, 4772-9	2.8	85
99	Improved SCF interaction energy decomposition scheme corrected for basis set superposition effect. *International Journal of Quantum Chemistry*, **1983**, 23, 847-854	2.1	83
98	Efficient techniques for the decomposition of intermolecular interaction energy at SCF level and beyond. *Computational and Theoretical Chemistry*, **1991**, 234, 387-400		73
97	Wide spectrum of H?H interactions: van der Waals contacts, dihydrogen bonds and covalency. *Chemical Physics*, **2007**, 337, 68-76	2.3	66
96	Insights into enzyme catalysis from QM/MM modelling: transition state stabilization in chorismate mutase. *Molecular Physics*, **2003**, 101, 2695-2714	1.7	66
95	Is a □□H+□□□ Complex Hydrogen Bonded?. *Journal of Physical Chemistry A*, **2004**, 108, 1806-1812	2.8	60
94	Are Various □Hole Bonds Steered by the Same Mechanisms?. *ChemPhysChem*, **2017**, 18, 1569-1577	3.2	59
93	Optimal methods for calculation of the amount of intermolecular electron transfer. *Journal of Chemical Physics*, **2002**, 117, 6952-6958	3.9	53

92	Computational study of the deamination reaction of cytosine with H2O and OH-. *Journal of Physical Chemistry A*, **2006**, 110, 8227-34	2.8	50
91	Can H□□H+□ and □H+□ interactions be classified as H-bonded?. *Chemical Physics Letters*, **2006**, 432, 33-39	2.5	50
90	Physical nature of ethidium and proflavine interactions with nucleic acid bases in the intercalation plane. *Journal of Physical Chemistry B*, **2006**, 110, 9720-7	3.4	49
89	Synthesis, and cytotoxic activity of some novel indolo[2,3-b]quinoline derivatives: DNA topoisomerase II inhibitors. *Bioorganic and Medicinal Chemistry*, **1999**, 7, 2457-64	3.4	49
88	Different types of hydrogen bonds: correlation analysis of interaction energy components. *Journal of Physical Organic Chemistry*, **2005**, 18, 779-784	2.1	48
87	Hydride bonding □Ab initio studies of BeH2□Li+, BeH2□Na+ and BeH2□Mg2+ model systems. *Chemical Physics Letters*, **2006**, 422, 334-339	2.5	46
86	Interaction energies in stacked DNA bases? How important are electrostatics?. *Chemical Physics Letters*, **2003**, 381, 729-732	2.5	44
85	New theoretical insight into the thermal cis□trans isomerization of azo compounds: Protonation lowers the activation barrier. *Journal of Chemical Physics*, **2001**, 114, 5504-5508	3.9	42
84	The physical nature of catalytic activity due to the molecular environment in terms of intermolecular interaction theory: derivation of simplified models. *Journal of Molecular Catalysis*, **1985**, 30, 395-410		42
83	The nature of interactions in the ionic crystal of 3-pentenenitrile, 2-nitro-5-oxo, ion(-1), sodium. *Journal of Physical Chemistry B*, **2005**, 109, 2027-33	3.4	36
82	Alkaline hydrolysis of organophosphorus pesticides: the dependence of the reaction mechanism on the incoming group conformation. *Journal of Physical Chemistry B*, **2014**, 118, 7277-89	3.4	34
81	Oxime-induced reactivation of sarin-inhibited AChE: a theoretical mechanisms study. *Journal of Physical Chemistry B*, **2007**, 111, 2404-8	3.4	33
80	Nonempirical Atom-Atom Potentials for Main Components of Intermolecular Interaction Energy. *Journal of Computational Chemistry*, **1986**, 7, 693-700	3.5	32
79	Attractive halogen□halogen interactions: F3CCl?FH and F3CCl?FCH3 dimers. *Chemical Physics*, **2006**, 327, 151-158	2.3	31
78	Intriguing relations of interaction energy components in stacked nucleic acids. *Journal of Chemical Physics*, **2007**, 127, 111102	3.9	30
77	Gas-phase mechanisms of degradation of hazardous organophosphorus compounds: do they follow a common pattern of alkaline hydrolysis reaction as in phosphotriesterase?. *Journal of Physical Chemistry B*, **2008**, 112, 9982-91	3.4	26
76	Cumulative atomic multipole moments complement any atomic charge model to obtain more accurate electrostatic properties. *Journal of Computational Chemistry*, **1992**, 13, 883-7	3.5	26
75	Improved procedure for analysis of electron density redistribution in molecular complexes. *Journal of Chemical Physics*, **1982**, 77, 4529-4541	3.9	26

74	Physical nature of intermolecular interactions within cAMP-dependent protein kinase active site: differential transition state stabilization in phosphoryl transfer reaction. *Journal of Physical Chemistry B*, **2008**, 112, 11819-26	3.4	25
73	Physical nature of interactions in charge-inverted hydrogen bonds. *Chemical Physics Letters*, **2012**, 552, 156-161	2.5	24
72	Nonempirical modeling of the static and dynamic properties of the optimum environment for chemical reactions. *Computational and Theoretical Chemistry*, **1986**, 138, 77-87		24
71	MM and QM/MM Modeling of Threonyl-tRNA Synthetase: Model Testing and Simulations. *Structural Chemistry*, **2004**, 15, 405-414	1.8	22
70	Efficient method for the generation and display of electrostatic potential surfaces from ab-initio wavefunctions. *Journal of Molecular Graphics*, **1991**, 9, 74-7, 94		22
69	Multipole correction of atomic monopole models of molecular charge distribution. I. Peptides. *Journal of Computational Chemistry*, **1993**, 14, 970-6	3.5	22
68	Theoretical model for exploration of catalytic activity of enzymes and design of new catalysts: CO2 hydration reaction. *International Journal of Quantum Chemistry*, **1981**, 20, 231-240	2.1	22
67	Understanding the role of carbamate reactivity in fatty acid amide hydrolase inhibition by QM/MM mechanistic modelling. *Chemical Communications*, **2011**, 47, 2517-9	5.8	21
66	Cumulative atomic multipole moments and point charge models describing molecular charge distribution. *Computer Physics Communications*, **1989**, 52, 397-408	4.2	21
65	Ab Initio Study of the Deamination of Formamidine. *Journal of Physical Chemistry A*, **2003**, 107, 11174-11181	2.81	20
64	The molecular basis of urokinase inhibition: from the nonempirical analysis of intermolecular interactions to the prediction of binding affinity. *Journal of Molecular Modeling*, **2007**, 13, 677-83	2	19
63	Origins of the activity of PAL and LAP enzyme inhibitors: toward ab initio binding affinity prediction. *Journal of the American Chemical Society*, **2005**, 127, 1658-9	16.4	19
62	Basis set extension effects on the He2 interaction energy components. *International Journal of Quantum Chemistry*, **1987**, 32, 279-293	2.1	19
61	Potential energy curves in complementary base pairs and in model hydrogen bonded systems. *International Journal of Quantum Chemistry*, **1981**, 20, 339-346	2.1	19
60	Approximate exchange perturbation study of intermolecular interactions in molecular complexes. *International Journal of Quantum Chemistry*, **1978**, 13, 679-692	2.1	19
59	Quantum chemical analysis of reaction paths in chorismate mutase: Conformational effects and electrostatic stabilization. *International Journal of Quantum Chemistry*, **2007**, 107, 2274-2285	2.1	18
58	Guidelines for development of basis sets for the first-order intermolecular interaction energy calculations. *Journal of Computational Chemistry*, **1983**, 4, 506-512	3.5	18
57	Double proton transfer and charge transfer transitions in hydrogen-bonded systems: formic acid dimer. *Chemical Physics Letters*, **1980**, 76, 88-91	2.5	18

56	Quantum chemical studies on molecular mechanism of mutations. *Advances in Molecular Relaxation and Interaction Processes*, **1977**, 11, 29-41		18
55	Analysis of the transferability of atomic multipoles for amino acids in modeling macromolecular charge distribution from fragments. *Journal of Computational Chemistry*, **2001**, 22, 1082-1097	3.5	17
54	Computer-aided design and activity prediction of leucine aminopeptidase inhibitors. *Journal of Computer-Aided Molecular Design*, **2000**, 14, 531-44	4.2	17
53	Procedure supplementing SCF interaction energies by dispersion term evaluated in dimer basis set within variation-perturbation approach. *Theoretica Chimica Acta*, **1986**, 70, 81-88		17
52	Basis set superposition effect on difference electrostatic molecular potential contour maps. *International Journal of Quantum Chemistry*, **1980**, 18, 165-171	2.1	16
51	Cumulative multicenter multipole moment databases and their applications. *Computational and Theoretical Chemistry*, **1992**, 256, 91-112		15
50	Robust Predictive Power of the Electrostatic Term at Shortened Intermolecular Distances. *Journal of Physical Chemistry Letters*, **2012**, 3, 2785-2789	6.4	13
49	Sequence-selectivity of 5,11-dimethyl-5H-indolo[2,3-b]quinoline binding to DNA. Footprinting and molecular modeling studies. *Bioorganic and Medicinal Chemistry*, **2000**, 8, 937-43	3.4	13
48	Non-empirical analysis of the nature of the inhibitor□active-site interactions in leucine aminopeptidase. *Chemical Physics Letters*, **1999**, 313, 385-392	2.5	13
47	Point charge representation of multicenter multipole moments in calculation of electrostatic properties. *Theoretica Chimica Acta*, **1993**, 85, 209-16		13
46	Molecular calculations with the nonempirical ab initioMODPOT, VRDDO, and MODPOT/VRDDO procedures. XI. Theoretical study of the [C6H5OH OC6H5]□molecular complex: Ab initioMODPOT/VRDDO calculations and electrostatic molecular potential contour maps. *International Journal of Quantum Chemistry*, **1980**, 18, 173-184	2.1	13
45	The Mechanism of Phosphoryl Transfer Reaction and the Role of Active Site Residues on the Basis of Ribokinase-Like Kinases. *International Journal of Molecular Sciences*, **2004**, 5, 141-153	6.3	12
44	Preliminary density functional calculations on the formic acid dimer. *Computers & Chemistry*, **1995**, 19, 181-187		12
43	Intramolecular electrostatic interactions studied by cumulative atomic multipole moment expansion with improved convergence. *Chemical Physics Letters*, **1994**, 221, 129-135	2.5	12
42	Physical nature of intermolecular interactions in [BMIM][PF6] ionic liquid. *Journal of Physical Chemistry B*, **2014**, 118, 2147-56	3.4	10
41	Nonempirical energetic analysis of reactivity and covalent inhibition of fatty acid amide hydrolase. *Journal of Physical Chemistry B*, **2013**, 117, 6656-66	3.4	10
40	Electrostatic nature of catalytic effects resulting from Si>Al substitutions in ZMS-5 zeolite. *Chemical Physics Letters*, **1998**, 288, 538-544	2.5	10
39	Physical nature of environmental effects on intermolecular proton transfer in (O2NOH?NH3)(H2O)n and (ClH?NH3)(H2O)n (n=1□) complexes. *Chemical Physics*, **2001**, 272, 37-45	2.3	10

38	POLY-CRYST A program for ab-initio crystal orbitals and polymer orbitals. *Journal of Non-Crystalline Solids*, **1985**, 75, 319-325	3.9	10
37	Rapid Estimation of Catalytic Efficiency by Cumulative Atomic Multipole Moments: Application to Ketosteroid Isomerase Mutants. *Journal of Chemical Theory and Computation*, **2017**, 13, 945-955	6.4	9
36	Quantum chemical analysis of the interactions of transition state analogs with leucine aminopeptidase. *International Journal of Quantum Chemistry*, **2001**, 84, 302-310	2.1	9
35	Cumulative atomic multipole moments for molecular crystals from ab-initio crystal orbital wave functions and for molecules in excited states from ab-initio MRD-CI wave functions. *International Journal of Quantum Chemistry*, **1990**, 38, 51-63	2.1	9
34	Physical Nature of Fatty Acid Amide Hydrolase Interactions with Its Inhibitors: Testing a Simple Nonempirical Scoring Model. *Journal of Physical Chemistry B*, **2014**, 118, 14727-36	3.4	8
33	Low cost prediction of relative stabilities of hydrogen bonded complexes from atomic multipole moments for overly short intermolecular distances. *Journal of Computational Chemistry*, **2013**, 34, 1797-9	3.5	8
32	The Ethidium-UA/AU Intercalation Site: Effect of Model Fragmentation and Backbone Charge State. *Journal of Chemical Theory and Computation*, **2011**, 7, 2600-9	6.4	8
31	Non-empirical study of the phosphorylation reaction catalyzed by 4-methyl-5-beta-hydroxyethylthiazole kinase: relevance of the theory of intermolecular interactions. *Journal of Molecular Modeling*, **2007**, 13, 839-49	2	8
30	Nonempirical analysis of the catalytic activity of the molecular environment Optimal static and dynamic catalytic fields for double proton transfer in formamideFormamidine complex. *Chemical Physics Letters*, **2003**, 367, 367-375	2.5	8
29	Nonempirical analysis of nature of catalytic effects in ribonuclease A active site. *Journal of Computational Chemistry*, **2000**, 21, 432-445	3.5	8
28	Bottom-Up Nonempirical Approach To Reducing Search Space in Enzyme Design Guided by Catalytic Fields. *Journal of Chemical Theory and Computation*, **2020**, 16, 3420-3429	6.4	8
27	Theoretical insights into catalysis by phosphonoacetaldehyde hydrolase. *Molecular Physics*, **2006**, 104, 2203-2211	1.7	7
26	DFT study of the reaction proceeding in the cytidine deaminase. *Chemical Physics Letters*, **2003**, 381, 660-665	2.5	7
25	Ab initio study of the physical nature of interactions between enzyme active site fragments invacuo. *Physical Chemistry Chemical Physics*, **2001**, 3, 657-663	3.6	7
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23	Interactions of 6-thioguanine in B-DNA: possible mechanism of its mutagenic action. *Journal of Theoretical Biology*, **1975**, 54, 167-74	2.3	7
22	Extreme Catalytic Power of Ketosteroid Isomerase Related to the Reversal of Proton Dislocations in Hydrogen-Bond Network. *Journal of Physical Chemistry B*, **2020**, 124, 3661-3666	3.4	7
21	Application of a simple quantum chemical approach to ligand fragment scoring for Trypanosoma brucei pteridine reductase1 inhibition. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 715-728	4.2	6

20	Universal short-range ab initio atom-atom potentials for interaction energy contributions with an optimal repulsion functional form. *Journal of Molecular Modeling*, **2015**, 21, 197	2	6
19	Theoretical studies on substrate binding to the active site of carbonic anhydrase. *International Journal of Quantum Chemistry*, **1979**, 16, 293-298	2.1	6
18	Tracking molecular charge distribution along reaction paths with atomic multipole moments. *Structural Chemistry*, **2016**, 27, 429-438	1.8	5
17	Ab initio multireference study of Hetero-Diels-Alder reaction of buta-1,3-diene with alkyl glyoxylates. *Journal of Molecular Modeling*, **2008**, 14, 727-33	2	5
16	Physical nature of interactions within the active site of cytosine-5-methyltransferase. *Journal of Physical Chemistry A*, **2006**, 110, 2308-13	2.8	5
15	Visualization of the Differential Transition State Stabilization within the Active Site Environment. *International Journal of Molecular Sciences*, **2004**, 5, 186-195	6.3	5
14	Correlated molecular and multicenter multipole moments in ground and excited states from multiple reference double-excitation configuration interaction calculations. *Journal of Computational Chemistry*, **1992**, 13, 944-951	3.5	5
13	Properties of the optimal environment inducing tautomerization of complementary base pairs. *Computational and Theoretical Chemistry*, **1987**, 150, 235-239		4
12	□AND □interactions in complementary bases. *Journal of Molecular Structure*, **1973**, 15, 263-271	3.4	4
11	Predicting substituent effects on activation energy changes by static catalytic fields. *Journal of Molecular Modeling*, **2017**, 24, 28	2	3
10	Libraries of atomic multipole moments for precise modeling of electrostatic properties of amino acids. *Amino Acids*, **1994**, 7, 19-26	3.5	3
9	Physical nature of catalytic effects of Si->Al substitutions in ZMS-5 zeolite for propylene protonation reaction. *Chemical Physics Letters*, **2002**, 364, 133-138	2.5	2
8	Environmentally Induced H-Bond Transformation as a Source of Anil□ype Molecule Specific Solvatochromy. *Molecular Crystals and Liquid Crystals*, **2005**, 427, 245/[557]-258/[570]	0.5	2
7	Catalytic Fields as a Tool to Analyze Enzyme Reaction Mechanism Variants and Reaction Steps. *Journal of Physical Chemistry B*, **2021**, 125, 11606-11616	3.4	2
6	The international workshop □Modeling & Design of Molecular Materials□held 16□20 September 2004 in Wroc□w. *Journal of Molecular Modeling*, **2005**, 11, 257-257	2	1
5	Usefulness of one electron properties in the study of the nitromethane-to-methyl nitrite rearrangement. *Journal of Molecular Graphics*, **1994**, 12, 207-11, 197		1
4	Explanation of the artifact structure predictions within the semiempirical ZDO SCF supermolecular approach. *International Journal of Quantum Chemistry*, **1980**, 18, 189-191	2.1	1
3	Programmable calculators. *Computers & Chemistry*, **1980**, 4, 165-177		1

2	Crystal structure studies using ab-initio potential functions from partitioned ab-initio MODPOT/VRDDO SCF energy calculations. I. N2 and CO2 test cases. II. Nitromethane, CH3NO2. *International Journal of Quantum Chemistry*, **2009**, 24, 375-391	2.1
1	From Inhibitors of Lap to Inhibitors of Pal. *Challenges and Advances in Computational Chemistry and Physics*, **2007**, 365-398	0.7