

# Waclaw Andrzej Sokalski

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Catalytic Fields as a Tool to Analyze Enzyme Reaction Mechanism Variants and Reaction Steps. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 11606-11616	3.4	2
108	Bottom-Up Nonempirical Approach To Reducing Search Space in Enzyme Design Guided by Catalytic Fields. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 3420-3429	6.4	8
107	Extreme Catalytic Power of Ketosteroid Isomerase Related to the Reversal of Proton Dislocations in Hydrogen-Bond Network. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 3661-3666	3.4	7
106	Rapid Estimation of Catalytic Efficiency by Cumulative Atomic Multipole Moments: Application to Ketosteroid Isomerase Mutants. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 945-955	6.4	9
105	Are Various $\pi$ -Hole Bonds Steered by the Same Mechanisms?. <i>ChemPhysChem</i> , <b>2017</b> , 18, 1569-1577	3.2	59
104	Predicting substituent effects on activation energy changes by static catalytic fields. <i>Journal of Molecular Modeling</i> , <b>2017</b> , 24, 28	2	3
103	Application of a simple quantum chemical approach to ligand fragment scoring for Trypanosoma brucei pteridine reductase $\beta$ inhibition. <i>Journal of Computer-Aided Molecular Design</i> , <b>2017</b> , 31, 715-728	4.2	6
102	Tracking molecular charge distribution along reaction paths with atomic multipole moments. <i>Structural Chemistry</i> , <b>2016</b> , 27, 429-438	1.8	5
101	Universal short-range ab initio atom-atom potentials for interaction energy contributions with an optimal repulsion functional form. <i>Journal of Molecular Modeling</i> , <b>2015</b> , 21, 197	2	6
100	Physical nature of intermolecular interactions in [BMIM][PF <sub>6</sub> ] ionic liquid. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 2147-56	3.4	10
99	Alkaline hydrolysis of organophosphorus pesticides: the dependence of the reaction mechanism on the incoming group conformation. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 7277-89	3.4	34
98	Physical Nature of Fatty Acid Amide Hydrolase Interactions with Its Inhibitors: Testing a Simple Nonempirical Scoring Model. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 14727-36	3.4	8
97	Nonempirical energetic analysis of reactivity and covalent inhibition of fatty acid amide hydrolase. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 6656-66	3.4	10
96	Low cost prediction of relative stabilities of hydrogen bonded complexes from atomic multipole moments for overly short intermolecular distances. <i>Journal of Computational Chemistry</i> , <b>2013</b> , 34, 1797-9	3.5	8
95	Robust Predictive Power of the Electrostatic Term at Shortened Intermolecular Distances. <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 2785-2789	6.4	13
94	Physical nature of interactions in charge-inverted hydrogen bonds. <i>Chemical Physics Letters</i> , <b>2012</b> , 552, 156-161	2.5	24
93	Understanding the role of carbamate reactivity in fatty acid amide hydrolase inhibition by QM/MM mechanistic modelling. <i>Chemical Communications</i> , <b>2011</b> , 47, 2517-9	5.8	21

92	The Ethidium-UA/AU Intercalation Site: Effect of Model Fragmentation and Backbone Charge State. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 2600-9	6.4	8
91	Crystal structure studies using ab-initio potential functions from partitioned ab-initio MODPOT/VRDDO SCF energy calculations. I. N <sub>2</sub> and CO <sub>2</sub> test cases. II. Nitromethane, CH <sub>3</sub> NO <sub>2</sub> . <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 24, 375-391	2.1	
90	Gas-phase mechanisms of degradation of hazardous organophosphorus compounds: do they follow a common pattern of alkaline hydrolysis reaction as in phosphotriesterase?. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 9982-91	3.4	26
89	Physical nature of intermolecular interactions within cAMP-dependent protein kinase active site: differential transition state stabilization in phosphoryl transfer reaction. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 11819-26	3.4	25
88	Ab initio multireference study of Hetero-Diels-Alder reaction of buta-1,3-diene with alkyl glyoxylates. <i>Journal of Molecular Modeling</i> , <b>2008</b> , 14, 727-33	2	5
87	Oxime-induced reactivation of sarin-inhibited AChE: a theoretical mechanisms study. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 2404-8	3.4	33
86	Wide spectrum of H?H interactions: van der Waals contacts, dihydrogen bonds and covalency. <i>Chemical Physics</i> , <b>2007</b> , 337, 68-76	2.3	66
85	Quantum chemical analysis of reaction paths in chorismate mutase: Conformational effects and electrostatic stabilization. <i>International Journal of Quantum Chemistry</i> , <b>2007</b> , 107, 2274-2285	2.1	18
84	Non-empirical study of the phosphorylation reaction catalyzed by 4-methyl-5-beta-hydroxyethylthiazole kinase: relevance of the theory of intermolecular interactions. <i>Journal of Molecular Modeling</i> , <b>2007</b> , 13, 839-49	2	8
83	The molecular basis of urokinase inhibition: from the nonempirical analysis of intermolecular interactions to the prediction of binding affinity. <i>Journal of Molecular Modeling</i> , <b>2007</b> , 13, 677-83	2	19
82	Intriguing relations of interaction energy components in stacked nucleic acids. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 111102	3.9	30
81	From Inhibitors of Lap to Inhibitors of Pal. <i>Challenges and Advances in Computational Chemistry and Physics</i> , <b>2007</b> , 365-398	0.7	
80	Physical nature of ethidium and proflavine interactions with nucleic acid bases in the intercalation plane. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 9720-7	3.4	49
79	Quantitative classification of covalent and noncovalent H-bonds. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 6444-6	3.4	197
78	Physical nature of interactions within the active site of cytosine-5-methyltransferase. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 2308-13	2.8	5
77	The possible covalent nature of N-H...O hydrogen bonds in formamide dimer and related systems: an ab initio study. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 4772-9	2.8	85
76	Computational study of the deamination reaction of cytosine with H <sub>2</sub> O and OH <sup>-</sup> . <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 8227-34	2.8	50
75	Theoretical insights into catalysis by phosphonoacetaldehyde hydrolase. <i>Molecular Physics</i> , <b>2006</b> , 104, 2203-2211	1.7	7

74	Attractive halogen-halogen interactions: F <sub>3</sub> CCl <sup>δ-</sup> FH and F <sub>3</sub> CCl <sup>δ-</sup> FCH <sub>3</sub> dimers. <i>Chemical Physics</i> , <b>2006</b> , 327, 151-158	2.3	31
73	Hydride bonding [Ab initio studies of BeH <sub>2</sub> Li <sup>+</sup> , BeH <sub>2</sub> Na <sup>+</sup> and BeH <sub>2</sub> Mg <sup>2+</sup> model systems. <i>Chemical Physics Letters</i> , <b>2006</b> , 422, 334-339	2.5	46
72	Can H <sup>δ+</sup> ...O <sup>δ-</sup> and H <sup>δ+</sup> ...N <sup>δ-</sup> interactions be classified as H-bonded?. <i>Chemical Physics Letters</i> , <b>2006</b> , 432, 33-39	2.5	50
71	The nature of interactions in the ionic crystal of 3-pentenenitrile, 2-nitro-5-oxo, ion(-1), sodium. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 2027-33	3.4	36
70	Origins of the activity of PAL and LAP enzyme inhibitors: toward ab initio binding affinity prediction. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 1658-9	16.4	19
69	How short can the H...H intermolecular contact be? New findings that reveal the covalent nature of extremely strong interactions. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 4331-41	2.8	172
68	The international workshop Modeling & Design of Molecular Materials held 16-20 September 2004 in Wrocław. <i>Journal of Molecular Modeling</i> , <b>2005</b> , 11, 257-257	2	1
67	Different types of hydrogen bonds: correlation analysis of interaction energy components. <i>Journal of Physical Organic Chemistry</i> , <b>2005</b> , 18, 779-784	2.1	48
66	Environmentally Induced H-Bond Transformation as a Source of Anil-type Molecule Specific Solvatochromy. <i>Molecular Crystals and Liquid Crystals</i> , <b>2005</b> , 427, 245/[557]-258/[570]	0.5	2
65	The Mechanism of Phosphoryl Transfer Reaction and the Role of Active Site Residues on the Basis of Ribokinase-Like Kinases. <i>International Journal of Molecular Sciences</i> , <b>2004</b> , 5, 141-153	6.3	12
64	Visualization of the Differential Transition State Stabilization within the Active Site Environment. <i>International Journal of Molecular Sciences</i> , <b>2004</b> , 5, 186-195	6.3	5
63	MM and QM/MM Modeling of Threonyl-tRNA Synthetase: Model Testing and Simulations. <i>Structural Chemistry</i> , <b>2004</b> , 15, 405-414	1.8	22
62	Is a H <sup>δ+</sup> ...C <sup>δ-</sup> Complex Hydrogen Bonded?. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 1806-1812	2.8	60
61	Nature of X <sup>δ-</sup> ...H <sup>δ+</sup> ...H <sup>δ+</sup> Dihydrogen Bonds and X <sup>δ-</sup> ...H <sup>δ+</sup> Interactions. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 5823-5830	2.8	87
60	Transition state stabilization and substrate strain in enzyme catalysis: ab initio QM/MM modelling of the chorismate mutase reaction. <i>Organic and Biomolecular Chemistry</i> , <b>2004</b> , 2, 968-80	3.9	94
59	Differential transition-state stabilization in enzyme catalysis: quantum chemical analysis of interactions in the chorismate mutase reaction and prediction of the optimal catalytic field. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 16148-59	16.4	88
58	Double-proton transfer in adenine-thymine and guanine-cytosine base pairs. A post-Hartree-Fock ab initio study. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 10119-29	16.4	185
57	DFT study of the reaction proceeding in the cytidine deaminase. <i>Chemical Physics Letters</i> , <b>2003</b> , 381, 660-665	2.5	7

56	Interaction energies in stacked DNA bases? How important are electrostatics?. <i>Chemical Physics Letters</i> , <b>2003</b> , 381, 729-732	2.5	44
55	Nonempirical analysis of the catalytic activity of the molecular environment [Optimal static and dynamic catalytic fields for double proton transfer in formamide-formamidinium complex. <i>Chemical Physics Letters</i> , <b>2003</b> , 367, 367-375	2.5	8
54	Ab Initio Study of the Deamination of Formamidinium. <i>Journal of Physical Chemistry A</i> , <b>2003</b> , 107, 11174-11181	2.5	20
53	Insights into enzyme catalysis from QM/MM modelling: transition state stabilization in chorismate mutase. <i>Molecular Physics</i> , <b>2003</b> , 101, 2695-2714	1.7	66
52	Physical nature of catalytic effects of Si->Al substitutions in ZMS-5 zeolite for propylene protonation reaction. <i>Chemical Physics Letters</i> , <b>2002</b> , 364, 133-138	2.5	2
51	Optimal methods for calculation of the amount of intermolecular electron transfer. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 6952-6958	3.9	53
50	Physical nature of environmental effects on intermolecular proton transfer in (O <sub>2</sub> NH <sup>+</sup> NH <sub>3</sub> )(H <sub>2</sub> O) <sub>n</sub> and (ClH <sup>+</sup> NH <sub>3</sub> )(H <sub>2</sub> O) <sub>n</sub> (n=1-3) complexes. <i>Chemical Physics</i> , <b>2001</b> , 272, 37-45	2.3	10
49	Quantum chemical analysis of the interactions of transition state analogs with leucine aminopeptidase. <i>International Journal of Quantum Chemistry</i> , <b>2001</b> , 84, 302-310	2.1	9
48	Analysis of the transferability of atomic multipoles for amino acids in modeling macromolecular charge distribution from fragments. <i>Journal of Computational Chemistry</i> , <b>2001</b> , 22, 1082-1097	3.5	17
47	New theoretical insight into the thermal cis-trans isomerization of azo compounds: Protonation lowers the activation barrier. <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 5504-5508	3.9	42
46	Ab initio study of the physical nature of interactions between enzyme active site fragments in vacuo. <i>Physical Chemistry Chemical Physics</i> , <b>2001</b> , 3, 657-663	3.6	7
45	Nonempirical analysis of nature of catalytic effects in ribonuclease A active site. <i>Journal of Computational Chemistry</i> , <b>2000</b> , 21, 432-445	3.5	8
44	Sequence-selectivity of 5,11-dimethyl-5H-indolo[2,3-b]quinoline binding to DNA. Footprinting and molecular modeling studies. <i>Bioorganic and Medicinal Chemistry</i> , <b>2000</b> , 8, 937-43	3.4	13
43	Computer-aided design and activity prediction of leucine aminopeptidase inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , <b>2000</b> , 14, 531-44	4.2	17
42	Synthesis, and cytotoxic activity of some novel indolo[2,3-b]quinoline derivatives: DNA topoisomerase II inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , <b>1999</b> , 7, 2457-64	3.4	49
41	Non-empirical analysis of the nature of the inhibitor-active-site interactions in leucine aminopeptidase. <i>Chemical Physics Letters</i> , <b>1999</b> , 313, 385-392	2.5	13
40	Electrostatic nature of catalytic effects resulting from Si->Al substitutions in ZMS-5 zeolite. <i>Chemical Physics Letters</i> , <b>1998</b> , 288, 538-544	2.5	10
39	Preliminary density functional calculations on the formic acid dimer. <i>Computers &amp; Chemistry</i> , <b>1995</b> , 19, 181-187		12

38	Libraries of atomic multipole moments for precise modeling of electrostatic properties of amino acids. <i>Amino Acids</i> , <b>1994</b> , 7, 19-26	3.5	3
37	Intramolecular electrostatic interactions studied by cumulative atomic multipole moment expansion with improved convergence. <i>Chemical Physics Letters</i> , <b>1994</b> , 221, 129-135	2.5	12
36	Usefulness of one electron properties in the study of the nitromethane-to-methyl nitrite rearrangement. <i>Journal of Molecular Graphics</i> , <b>1994</b> , 12, 207-11, 197		1
35	Multipole correction of atomic monopole models of molecular charge distribution. I. Peptides. <i>Journal of Computational Chemistry</i> , <b>1993</b> , 14, 970-6	3.5	22
34	Point charge representation of multicenter multipole moments in calculation of electrostatic properties. <i>Theoretica Chimica Acta</i> , <b>1993</b> , 85, 209-16		13
33	Cumulative multicenter multipole moment databases and their applications. <i>Computational and Theoretical Chemistry</i> , <b>1992</b> , 256, 91-112		15
32	Cumulative atomic multipole moments complement any atomic charge model to obtain more accurate electrostatic properties. <i>Journal of Computational Chemistry</i> , <b>1992</b> , 13, 883-7	3.5	26
31	Correlated molecular and multicenter multipole moments in ground and excited states from multiple reference double-excitation configuration interaction calculations. <i>Journal of Computational Chemistry</i> , <b>1992</b> , 13, 944-951	3.5	5
30	Efficient method for the generation and display of electrostatic potential surfaces from ab-initio wavefunctions. <i>Journal of Molecular Graphics</i> , <b>1991</b> , 9, 74-7, 94		22
29	Efficient techniques for the decomposition of intermolecular interaction energy at SCF level and beyond. <i>Computational and Theoretical Chemistry</i> , <b>1991</b> , 234, 387-400		73
28	Catalytic activity of aminoacyl tRNA synthetases and its implications for the origin of life. I. Aminoacyl adenylate formation in tyrosyl tRNA synthetase. <i>Journal of Molecular Evolution</i> , <b>1991</b> , 33, 405-11	3.1	7
27	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. <i>International Journal of Quantum Chemistry</i> , <b>1990</b> , 38, 51-63	2.1	9
26	Cumulative atomic multipole moments and point charge models describing molecular charge distribution. <i>Computer Physics Communications</i> , <b>1989</b> , 52, 397-408	4.2	21
25	An efficient procedure for decomposition of the SCF interaction energy into components with reduced basis set dependence. <i>Chemical Physics Letters</i> , <b>1988</b> , 153, 153-159	2.5	187
24	Correlated molecular and cumulative atomic multipole moments. <i>Journal of Chemical Physics</i> , <b>1987</b> , 87, 526-534	3.9	101
23	Properties of the optimal environment inducing tautomerization of complementary base pairs. <i>Computational and Theoretical Chemistry</i> , <b>1987</b> , 150, 235-239		4
22	Basis set extension effects on the He <sub>2</sub> interaction energy components. <i>International Journal of Quantum Chemistry</i> , <b>1987</b> , 32, 279-293	2.1	19
21	Nonempirical Atom-Atom Potentials for Main Components of Intermolecular Interaction Energy. <i>Journal of Computational Chemistry</i> , <b>1986</b> , 7, 693-700	3.5	32



20	Procedure supplementing SCF interaction energies by dispersion term evaluated in dimer basis set within variation-perturbation approach. <i>Theoretica Chimica Acta</i> , <b>1986</b> , 70, 81-88		17
19	Nonempirical modeling of the static and dynamic properties of the optimum environment for chemical reactions. <i>Computational and Theoretical Chemistry</i> , <b>1986</b> , 138, 77-87		24
18	The physical nature of catalytic activity due to the molecular environment in terms of intermolecular interaction theory: derivation of simplified models. <i>Journal of Molecular Catalysis</i> , <b>1985</b> , 30, 395-410		42
17	POLY-CRYST I A program for ab-initio crystal orbitals and polymer orbitals. <i>Journal of Non-Crystalline Solids</i> , <b>1985</b> , 75, 319-325	3.9	10
16	Improved SCF interaction energy decomposition scheme corrected for basis set superposition effect. <i>International Journal of Quantum Chemistry</i> , <b>1983</b> , 23, 847-854	2.1	83
15	Guidelines for development of basis sets for the first-order intermolecular interaction energy calculations. <i>Journal of Computational Chemistry</i> , <b>1983</b> , 4, 506-512	3.5	18
14	Cumulative atomic multipole representation of the molecular charge distribution and its basis set dependence. <i>Chemical Physics Letters</i> , <b>1983</b> , 98, 86-92	2.5	187
13	Improved procedure for analysis of electron density redistribution in molecular complexes. <i>Journal of Chemical Physics</i> , <b>1982</b> , 77, 4529-4541	3.9	26
12	Theoretical model for exploration of catalytic activity of enzymes and design of new catalysts: CO <sub>2</sub> hydration reaction. <i>International Journal of Quantum Chemistry</i> , <b>1981</b> , 20, 231-240	2.1	22
11	Potential energy curves in complementary base pairs and in model hydrogen bonded systems. <i>International Journal of Quantum Chemistry</i> , <b>1981</b> , 20, 339-346	2.1	19
10	Double proton transfer and charge transfer transitions in hydrogen-bonded systems: formic acid dimer. <i>Chemical Physics Letters</i> , <b>1980</b> , 76, 88-91	2.5	18
9	Basis set superposition effect on difference electrostatic molecular potential contour maps. <i>International Journal of Quantum Chemistry</i> , <b>1980</b> , 18, 165-171	2.1	16
8	Molecular calculations with the nonempirical ab initio MODPOT, VRDDO, and MODPOT/VRDDO procedures. XI. Theoretical study of the [C <sub>6</sub> H <sub>5</sub> OH...OC <sub>6</sub> H <sub>5</sub> ] <sup>+</sup> molecular complex: Ab initio MODPOT/VRDDO calculations and electrostatic molecular potential contour maps. <i>International Journal of Quantum Chemistry</i> , <b>1980</b> , 18, 173-184	2.1	13
7	Explanation of the artifact structure predictions within the semiempirical ZDO SCF supermolecular approach. <i>International Journal of Quantum Chemistry</i> , <b>1980</b> , 18, 189-191	2.1	1
6	Programmable calculators. <i>Computers &amp; Chemistry</i> , <b>1980</b> , 4, 165-177		1
5	Theoretical studies on substrate binding to the active site of carbonic anhydrase. <i>International Journal of Quantum Chemistry</i> , <b>1979</b> , 16, 293-298	2.1	6
4	Approximate exchange perturbation study of intermolecular interactions in molecular complexes. <i>International Journal of Quantum Chemistry</i> , <b>1978</b> , 13, 679-692	2.1	19
3	Quantum chemical studies on molecular mechanism of mutations. <i>Advances in Molecular Relaxation and Interaction Processes</i> , <b>1977</b> , 11, 29-41		18

- 2 Interactions of 6-thioguanine in B-DNA: possible mechanism of its mutagenic action. *Journal of Theoretical Biology*, **1975**, 54, 167-74 2-3 7
- 1  $\pi$ - $\pi$  AND  $\pi$ - $\pi$  interactions in complementary bases. *Journal of Molecular Structure*, **1973**, 15, 263-271 3-4 4