Waclaw Andrzej Sokalski

List of Publications by Year
in descending order

114 papers	3,667 citations	147566 31 h-index	143772 57 g-index
117 all docs	117 docs citations	117 times ranked	2264 citing authors

#	Article	IF	Citations
1	Quantitative Classification of Covalent and Noncovalent H-Bonds. Journal of Physical Chemistry B, 2006, 110, 6444-6446.	1.2	224
2	An efficient procedure for decomposition of the SCF interaction energy into components with reduced basis set dependence. Chemical Physics Letters, 1988, 153, 153-159.	1.2	205
3	Double-Proton Transfer in Adenineâ^'Thymine and Guanineâ^'Cytosine Base Pairs. A Post-Hartreeâ^'Fock ab Initio Study. Journal of the American Chemical Society, 2004, 126, 10119-10129.	6.6	201
4	Cumulative atomic multipole representation of the molecular charge distribution and its basis set dependence. Chemical Physics Letters, 1983, 98, 86-92.	1.2	196
5	How Short Can the HÂ·Â·Â·H Intermolecular Contact Be? New Findings that Reveal the Covalent Nature of Extremely Strong Interactions. Journal of Physical Chemistry A, 2005, 109, 4331-4341.	1.1	188
6	Correlated molecular and cumulative atomic multipole moments. Journal of Chemical Physics, 1987, 87, 526-534.	1.2	106
7	Differential Transition-State Stabilization in Enzyme Catalysis:Â 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, 16148-16159.	6.6	104
8	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.	1.5	98
9	Nature of Xâ^'H+Î^Â·Â·Â·Î^Hâ^'Y Dihydrogen Bonds and Xâ^'HÂ·Â·Â·Ïƒ Interactions. Journal of Physical Chemistry A, 2004, 108, 5823-5830.	1.1	93
10	The Possible Covalent Nature of Nâ^'HÂ·Â·Â·O Hydrogen Bonds in Formamide Dimer and Related Systems:Â An Ab Initio Study. Journal of Physical Chemistry A, 2006, 110, 4772-4779.	1.1	90
11	ImprovedSCF interaction energy decomposition scheme corrected for basis set superposition effect. International Journal of Quantum Chemistry, 1983, 23, 847-854.	1.0	84
12	Efficient techniques for the decomposition of intermolecular interaction energy at SCF level and beyond. Computational and Theoretical Chemistry, 1991, 234, 387-400.	1.5	82
13	Wide spectrum of Hâ‹¯H interactions: van der Waals contacts, dihydrogen bonds and covalency. Chemical Physics, 2007, 337, 68-76.	0.9	74
14	Insights into enzyme catalysis from QM/MM modelling: transition state stabilization in chorismate mutase. Molecular Physics, 2003, 101, 2695-2714.	0.8	73
15	Is a Ï€Â·Â·Â·H+Â·Â·Â·Ï€ Complex Hydrogen Bonded?. Journal of Physical Chemistry A, 2004, 108, 1806-1812.	1.1	68
16	Are Various Ïƒâ€Hole Bonds Steered by the Same Mechanisms?. ChemPhysChem, 2017, 18, 1569-1577.	1.0	67
17	Synthesis, and cytotoxic activity of some novel indolo[2,3-b]quinoline derivatives. Bioorganic and Medicinal Chemistry, 1999, 7, 2457-2464.	1.4	57
18	Computational Study of the Deamination Reaction of Cytosine with H2O and OH-. Journal of Physical Chemistry A, 2006, 110, 8227-8234.	1.1	56

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19	Can Hâ€¦Ïƒ, Ï€â€¦H+â€¦Ïƒ and Ïƒâ€¦H+â€¦Ïƒ interactions be classified as H-bonded?. Chemical Physics Letters, 2006, 432, 33-39.	1.2	55
20	Different types of hydrogen bonds: correlation analysis of interaction energy components. Journal of Physical Organic Chemistry, 2005, 18, 779-784.	0.9	54
21	Optimal methods for calculation of the amount of intermolecular electron transfer. Journal of Chemical Physics, 2002, 117, 6952-6958.	1.2	53
22	Physical Nature of Ethidium and Proflavine Interactions with Nucleic Acid Bases in the Intercalation Plane. Journal of Physical Chemistry B, 2006, 110, 9720-9727.	1.2	53
23	Hydride bonding â€“ Ab initio studies of BeH2â€¦Li+, BeH2â€¦Na+ and BeH2â€¦Mg2+ model systems. Chemical Physics Letters, 2006, 422, 334-339.	1.2	52
24	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.	1.2	49
25	New theoretical insight into the thermal cisâ€“trans isomerization of azo compounds: Protonation lowers the activation barrier. Journal of Chemical Physics, 2001, 114, 5504-5508.	1.2	49
26	Interaction energies in stacked DNA bases? How important are electrostatics?. Chemical Physics Letters, 2003, 381, 729-732.	1.2	45
27	Alkaline Hydrolysis of Organophosphorus Pesticides: The Dependence of the Reaction Mechanism on the Incoming Group Conformation. Journal of Physical Chemistry B, 2014, 118, 7277-7289.	1.2	43
28	The Nature of Interactions in the Ionic Crystal of 3-Pentenenitrile, 2-Nitro-5-oxo, Ion(â^'1), Sodium. Journal of Physical Chemistry B, 2005, 109, 2027-2033.	1.2	38
29	Oxime-Induced Reactivation of Sarin-Inhibited AChE:Â A Theoretical Mechanisms Study. Journal of Physical Chemistry B, 2007, 111, 2404-2408.	1.2	37
30	Nonempirical Atom-Atom Potentials for Main Components of Intermolecular Interaction Energy. Journal of Computational Chemistry, 1986, 7, 693-700.	1.5	34
31	Attractive halogenâ€“halogen interactions: F3CClâ‹¯FH and F3CClâ‹¯FCH3 dimers. Chemical Physics, 2006, 327, 151-158.	0.9	34
32	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, 11819-11826.	1.2	32
33	Intriguing relations of interaction energy components in stacked nucleic acids. Journal of Chemical Physics, 2007, 127, 111102.	1.2	31
34	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, 9982-9991.	1.2	31
35	Understanding the role of carbamate reactivity in fatty acid amide hydrolase inhibition by QM/MM mechanistic modelling. Chemical Communications, 2011, 47, 2517.	2.2	29
36	Improved procedure for analysis of electron density redistribution in molecular complexes. Journal of Chemical Physics, 1982, 77, 4529-4541.	1.2	28

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37	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.	1.0	27
38	Cumulative atomic multipole moments complement any atomic charge model to obtain more accurate electrostatic properties. Journal of Computational Chemistry, 1992, 13, 883-887.	1.5	26
39	Physical nature of interactions in charge-inverted hydrogen bonds. Chemical Physics Letters, 2012, 552, 156-161.	1.2	26
40	Nonempirical modeling of the static and dynamic properties of the optimum environment for chemical reactions. Computational and Theoretical Chemistry, 1986, 138, 77-87.	1.5	25
41	Efficient method for the generation and display of electrostatic potential surfaces from ab-initio wavefunctions. Journal of Molecular Graphics, 1991, 9, 74-77.	1.7	22
42	Multipole correction of atomic monopole models of molecular charge distribution. I. Peptides. Journal of Computational Chemistry, 1993, 14, 970-976.	1.5	22
43	MM and QM/MM Modeling of Threonyl-tRNA Synthetase: Model Testing and Simulations. Structural Chemistry, 2004, 15, 405-414.	1.0	22
44	Potential energy curves in complementary base pairs and in model hydrogen bonded systems. International Journal of Quantum Chemistry, 1981, 20, 339-346.	1.0	21
45	Cumulative atomic multipole moments and point charge models describing molecular charge distribution. Computer Physics Communications, 1989, 52, 397-408.	3.0	21
46	Approximate exchange perturbation study of intermolecular interactions in molecular complexes. International Journal of Quantum Chemistry, 1978, 13, 679-692.	1.0	20
47	Basis set extension effects on the He2 interaction energy components. International Journal of Quantum Chemistry, 1987, 32, 279-293.	1.0	20
48	Ab Initio Study of the Deamination of Formamidine. Journal of Physical Chemistry A, 2003, 107, 11174-11181.	1.1	20
49	Origins of the Activity of PAL and LAP Enzyme Inhibitors:Â Toward Ab Initio Binding Affinity Prediction. Journal of the American Chemical Society, 2005, 127, 1658-1659.	6.6	20
50	Quantum chemical analysis of reaction paths in chorismate mutase: Conformational effects and electrostatic stabilization. International Journal of Quantum Chemistry, 2007, 107, 2274-2285.	1.0	20
51	Quantum chemical studies on molecular mechanism of mutations. Advances in Molecular Relaxation and Interaction Processes, 1977, 11, 29-41.	0.6	19
52	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, 677-683.	0.8	19
53	Double proton transfer and charge transfer transitions in hydrogen-bonded systems: formic acid dimer. Chemical Physics Letters, 1980, 76, 88-91.	1.2	18
54	Guidelines for development of basis sets for the first-order intermolecular interaction energy calculations. Journal of Computational Chemistry, 1983, 4, 506-512.	1.5	18

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55	Computer-aided design and activity prediction of leucine aminopeptidase inhibitors. Journal of Computer-Aided Molecular Design, 2000, 14, 531-544.	1.3	18
56	Procedure supplementing SCF interaction energies by dispersion term evaluated in dimer basis set within variation-perturbation approach. Theoretica Chimica Acta, 1986, 70, 81-88.	0.9	17
57	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.	1.5	17
58	Basis set superposition effect on difference electrostatic molecular potential contour maps. International Journal of Quantum Chemistry, 1980, 18, 165-171.	1.0	16
59	Cumulative multicenter multipole moment databases and their applications. Computational and Theoretical Chemistry, 1992, 256, 91-112.	1.5	15
60	Non-empirical analysis of the nature of the inhibitorâ€“active-site interactions in leucine aminopeptidase. Chemical Physics Letters, 1999, 313, 385-392.	1.2	15
61	Robust Predictive Power of the Electrostatic Term at Shortened Intermolecular Distances. Journal of Physical Chemistry Letters, 2012, 3, 2785-2789.	2.1	15
62	Intramolecular electrostatic interactions studied by cumulative atomic multipole moment expansion with improved convergence. Chemical Physics Letters, 1994, 221, 129-135.	1.2	14
63	Sequence-selectivity of 5,11-dimethyl-5 H -indolo[2,3- b]quinoline binding to DNA. Footprinting and molecular modeling studies. Bioorganic and Medicinal Chemistry, 2000, 8, 937-943.	1.4	14
64	Molecular calculations with the nonempiricalab initioMODPOT,VRDDO, andMODPOT/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.	1.0	13
65	Point charge representation of multicenter multipole moments in calculation of electrostatic properties. Theoretica Chimica Acta, 1993, 85, 209-216.	0.9	13
66	Preliminary density functional calculations on the formic acid dimer. Computers & Chemistry, 1995, 19, 181-187.	1.2	13
67	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.	1.8	12
68	Electrostatic nature of catalytic effects resulting from Si>Al substitutions in ZMS-5 zeolite. Chemical Physics Letters, 1998, 288, 538-544.	1.2	11
69	Nonempirical Energetic Analysis of Reactivity and Covalent Inhibition of Fatty Acid Amide Hydrolase. Journal of Physical Chemistry B, 2013, 117, 6656-6666.	1.2	11
70	POLY-CRYST â€" A program for ab-initio crystal orbitals and polymer orbitals. Journal of Non-Crystalline Solids, 1985, 75, 319-325.	1.5	10
71	Cumulative atomic multipole moments for molecular crystals fromab-initio crystal orbital wave functions and for molecules in excited states fromab-initio MRD-CI wave functions. International Journal of Quantum Chemistry, 1990, 38, 51-63.	1.0	10
72	Physical nature of environmental effects on intermolecular proton transfer in (O2NOHâ‹¯NH3)(H2O)n and (ClHâ‹¯NH3)(H2O)n (n=1â€“3) complexes. Chemical Physics, 2001, 272, 37-45.	0.9	10

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73	Physical Nature of Intermolecular Interactions in [BMIM][PF₆] Ionic Liquid. Journal of Physical Chemistry B, 2014, 118, 2147-2156.	1.2	10
74	Nonempirical analysis of nature of catalytic effects in ribonuclease A active site. Journal of Computational Chemistry, 2000, 21, 432-445.	1.5	9
75	Quantum chemical analysis of the interactions of transition state analogs with leucine aminopeptidase. International Journal of Quantum Chemistry, 2001, 84, 302-310.	1.0	9
76	Physical Nature of Fatty Acid Amide Hydrolase Interactions with Its Inhibitors: Testing a Simple Nonempirical Scoring Model. Journal of Physical Chemistry B, 2014, 118, 141210162534006.	1.2	9
77	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.	2.3	9
78	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.	2.3	9
79	Theoretical studies on substrate binding to the active site of carbonic anhydrase. International Journal of Quantum Chemistry, 1979, 16, 293-298.	1.0	8
80	Nonempirical analysis of the catalytic activity of the molecular environment â€“ optimal static and dynamic catalytic fields for double proton transfer in formamideâ€“formamidine complex. Chemical Physics Letters, 2003, 367, 367-375.	1.2	8
81	Theoretical insights into catalysis by phosphonoacetaldehyde hydrolase. Molecular Physics, 2006, 104, 2203-2211.	0.8	8
82	Non-empirical study of the phosphorylation reaction catalyzed by 4-methyl-5-Î²-hydroxyethylthiazole kinase: relevance of the theory of intermolecular interactions. Journal of Molecular Modeling, 2007, 13, 839-849.	0.8	8
83	The Ethidiumâ€“UA/AU Intercalation Site: Effect of Model Fragmentation and Backbone Charge State. Journal of Chemical Theory and Computation, 2011, 7, 2600-2609.	2.3	8
84	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, 1797-1799.	1.5	8
85	Application of a simple quantum chemical approach to ligand fragment scoring for Trypanosoma brucei pteridine reductaseÂ1 inhibition. Journal of Computer-Aided Molecular Design, 2017, 31, 715-728.	1.3	8
86	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.	1.2	8
87	Interactions of 6-thioguanine in B-DNA: Possible mechanism of its mutagenic action. Journal of Theoretical Biology, 1975, 54, 167-174.	0.8	7
88	Catalytic activity of aminoacyl tRNA synthetases and its implications for the origin of life. I. Aminoacyl adenylate formation in tyrosyl tRNA synthetase. Journal of Molecular Evolution, 1991, 33, 405-411.	0.8	7
89	Ab initio study of the physical nature of interactions between enzyme active site fragments in vacuo. Physical Chemistry Chemical Physics, 2001, 3, 657-663.	1.3	7
90	DFT study of the reaction proceeding in the cytidine deaminase. Chemical Physics Letters, 2003, 381, 660-665.	1.2	7

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91	Catalytic Fields as a Tool to Analyze Enzyme Reaction Mechanism Variants and Reaction Steps. Journal of Physical Chemistry B, 2021, 125, 11606-11616.	1.2	7
92	Visualization of the Differential Transition State Stabilization within the Active Site Environment. International Journal of Molecular Sciences, 2004, 5, 186-195.	1.8	6
93	Universal short-range ab initio atomâ€“atom potentials for interaction energy contributions with an optimal repulsion functional form. Journal of Molecular Modeling, 2015, 21, 197.	0.8	6
94	Tracking molecular charge distribution along reaction paths with atomic multipole moments. Structural Chemistry, 2016, 27, 429-438.	1.0	6
95	Properties of the optimal environment inducing tautomerization of complementary base pairs. Computational and Theoretical Chemistry, 1987, 150, 235-239.	1.5	5
96	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.	1.5	5
97	Physical Nature of Interactions within the Active Site of Cytosine-5-methyltransferase. Journal of Physical Chemistry A, 2006, 110, 2308-2313.	1.1	5
98	Ab initio multireference study of Hetero-Diels-Alder reaction of buta-1,3-diene with alkyl glyoxylates. Journal of Molecular Modeling, 2008, 14, 727-733.	0.8	5
99	Ïƒ-Ïƒ AND Ï€-Ï€ interactions in complementary bases. Journal of Molecular Structure, 1973, 15, 263-271.	1.8	4
100	Libraries of atomic multipole moments for precise modeling of electrostatic properties of amino acids. Amino Acids, 1994, 7, 19-26.	1.2	4
101	Predicting substituent effects on activation energy changes by static catalytic fields. Journal of Molecular Modeling, 2018, 24, 28.	0.8	3
102	Explanation of the artifact structure predictions within the semiempiricalZDO SCF supermolecular approach. International Journal of Quantum Chemistry, 1980, 18, 189-191.	1.0	2
103	Physical nature of catalytic effects of Siâ†'Al substitutions in ZMS-5 zeolite for propylene protonation reaction. Chemical Physics Letters, 2002, 364, 133-138.	1.2	2
104	The international workshop â€œModeling & Design of Molecular Materialsâ€, held 16â€“20 September 2004 in WrocÅ‚aw. Journal of Molecular Modeling, 2005, 11, 257-257.	0.8	2
105	Environmentally Induced H-Bond Transformation as a Source of Anilâ€“Type Molecule Specific Solvatochromy. Molecular Crystals and Liquid Crystals, 2005, 427, 245/[557]-258/[570].	0.4	2
106	Programmable calculators. Computers & Chemistry, 1980, 4, 165-177.	1.2	1
107	Usefulness of one electron properties in the study of the nitromethane-to-methyl nitrite rearrangement. Journal of Molecular Graphics, 1994, 12, 207-211.	1.7	1
108	From Inhibitors of Lap to Inhibitors of Pal. Challenges and Advances in Computational Chemistry and Physics, 2007, , 365-398.	0.6	1

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109	How Short Can the HÃ—Ã—Ã—H Intermolecular Contact Be? New Findings that Reveal the Covalent Nature of Extremely Strong Interactions.. ChemInform, 2005, 36, no.	0.1	0
110	International conference and workshop: Modeling and Design of Molecular Materials (10â€“15) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 70	0.8	0
111	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.	1.0	0
112	International conference: Modeling and Design of Molecular Materialsâ€”MDMM 2010 (4â€“8 July 2010,) Tj ETQq0 0 0 rgBT /Overlock 1	0.8	0
113	International conference: Modeling & Design of Molecular Materialsâ€”MDMM 2012 (September 10â€“14,) Tj ETQq1 1 0.784314 rgBT	0.8	0
114	The international workshop â€œModeling & Design of Molecular Materialsâ€, held 16â€“20 September 2004 in WrocÅ‚aw. Journal of Molecular Modeling, 0, , .	0.8	0