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List of Publications by Year in Descending Order

102 papers	12,008 citations	39 h-index	109 g-index
111 ext. papers	13,548 ext. citations	3.8 avg, IF	6.01 L-index

#	Paper	IF	Citations
102	Molecule-surface interaction from van der Waals-corrected semilocal density functionals: The example of thiophene on transition-metal surfaces. *Physical Review Materials*, **2020**, 4,	3.2	12
101	Simple Modifications of the SCAN Meta-Generalized Gradient Approximation Functional. *Journal of Chemical Theory and Computation*, **2018**, 14, 2469-2479	6.4	23
100	Reference Determinant Dependence of the Random Phase Approximation in 3d Transition Metal Chemistry. *Journal of Chemical Theory and Computation*, **2017**, 13, 100-109	6.4	13
99	Construction of a Spin-Component Scaled Dual-Hybrid Random Phase Approximation. *Journal of Chemical Theory and Computation*, **2017**, 13, 796-803	6.4	23
98	Electron Density Errors and Density-Driven Exchange-Correlation Energy Errors in Approximate Density Functional Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 4753-4764	6.4	33
97	Features of the interactions between the methyl-CpG motif and the arginine residues on the surface of MBD proteins. *Structural Chemistry*, **2016**, 27, 1317-1326	1.8	5
96	Why Density Functionals Should Not Be Judged Primarily by Atomization Energies. *Periodica Polytechnica: Chemical Engineering*, **2016**, 60, 2-7	1.3	17
95	Application of a Dual-Hybrid Direct Random Phase Approximation to Water Clusters. *Journal of Chemical Theory and Computation*, **2016**, 12, 4222-32	6.4	7
94	Accurate Complete Basis Set Extrapolation of Direct Random Phase Correlation Energies. *Journal of Chemical Theory and Computation*, **2015**, 11, 3961-7	6.4	9
93	Accurate Diels-Alder reaction energies from efficient density functional calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 2879-88	6.4	17
92	Construction and application of a new dual-hybrid random phase approximation. *Journal of Chemical Theory and Computation*, **2015**, 11, 4615-26	6.4	48
91	Accurate, precise, and efficient theoretical methods to calculate anion-□interaction energies in model structures. *Journal of Chemical Theory and Computation*, **2015**, 11, 360-71	6.4	23
90	Unified picture for the conformation and stabilization of the O-glycosidic linkage in glycopeptide model structures. *Structural Chemistry*, **2015**, 26, 1367-1376	1.8	5
89	Density functionals that recognize covalent, metallic, and weak bonds. *Physical Review Letters*, **2013**, 111, 106401	7.4	143
88	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2013**, 9, 355-63	6.4	62
87	van der Waals interaction as a summable asymptotic series. *Physical Review A*, **2012**, 86,	2.6	15
86	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. *Journal of Physics Condensed Matter*, **2012**, 24, 424207	1.8	12

85	Van der waals coefficients for nanostructures: fullerenes defy conventional wisdom. *Physical Review Letters*, **2012**, 109, 233203	7.4	62
84	A meta-GGA Made Free of the Order of Limits Anomaly. *Journal of Chemical Theory and Computation*, **2012**, 8, 2078-87	6.4	44
83	Lattice constants from semilocal density functionals with zero-point phonon correction. *Physical Review B*, **2012**, 85,	3.3	52
82	Conformational analysis of cellobiose by electronic structure theories. *Carbohydrate Research*, **2012**, 350, 68-76	2.9	46
81	Accurate Conformational Energy Differences of Carbohydrates: A Complete Basis Set Extrapolation. *Journal of Chemical Theory and Computation*, **2011**, 7, 988-97	6.4	21
80	Hydroxyl orientations in cellobiose and other polyhydroxyl compounds: modeling versus experiment. *Cellulose*, **2011**, 18, 897-909	5.5	18
79	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. *Physical Review B*, **2011**, 84,	3.3	138
78	A simple but fully nonlocal correction to the random phase approximation. *Journal of Chemical Physics*, **2011**, 134, 114110	3.9	31
77	Global Hybrid Functionals: A Look at the Engine under the Hood. *Journal of Chemical Theory and Computation*, **2010**, 6, 3688-3703	6.4	77
76	The RPA Atomization Energy Puzzle. *Journal of Chemical Theory and Computation*, **2010**, 6, 127-34	6.4	70
75	Comparison of different force fields for the study of disaccharides. *Carbohydrate Research*, **2009**, 344, 2217-28	2.9	78
74	Evaluation of Density Functionals and Basis Sets for Carbohydrates. *Journal of Chemical Theory and Computation*, **2009**, 5, 679-92	6.4	157
73	Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. *Journal of Chemical Theory and Computation*, **2009**, 5, 2950-8	6.4	70
72	Regularized Gradient Expansion for Atoms, Molecules, and Solids. *Journal of Chemical Theory and Computation*, **2009**, 5, 763-9	6.4	34
71	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. *Journal of Chemical Theory and Computation*, **2009**, 5, 902-8	6.4	273
70	Workhorse semilocal density functional for condensed matter physics and quantum chemistry. *Physical Review Letters*, **2009**, 103, 026403	7.4	426
69	Assessing the performance of recent density functionals for bulk solids. *Physical Review B*, **2009**, 79,	3.3	530
68	Perdew et al. Reply:. *Physical Review Letters*, **2008**, 101,	7.4	55

67	Improved Description of Stereoelectronic Effects in Hydrocarbons Using Semilocal Density Functional Theory. *Journal of Chemical Theory and Computation*, **2008**, 4, 888-91	6.4	55
66	Simple charge-transfer model to explain the electrical response of hydrogen chains. *Physical Review A*, **2008**, 78,	2.6	19
65	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. *Physical Review A*, **2008**, 77,	2.6	48
64	Restoring the density-gradient expansion for exchange in solids and surfaces. *Physical Review Letters*, **2008**, 100, 136406	7.4	5934
63	Exchange and correlation in open systems of fluctuating electron number. *Physical Review A*, **2007**, 76,	2.6	131
62	Density functionals that are one- and two- are not always many-electron self-interaction-free, as shown for H2+, He2+, LiH+, and Ne2+. *Journal of Chemical Physics*, **2007**, 126, 104102	3.9	248
61	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. *Physical Review A*, **2007**, 76,	2.6	37
60	Diminished gradient dependence of density functionals: constraint satisfaction and self-interaction correction. *Journal of Chemical Physics*, **2007**, 126, 244107	3.9	25
59	Meta-generalized gradient approximation: non-empirical construction and performance of a density functional. *Philosophical Magazine*, **2007**, 87, 1071-1084	1.6	11
58	Spurious fractional charge on dissociated atoms: pervasive and resilient self-interaction error of common density functionals. *Journal of Chemical Physics*, **2006**, 125, 194112	3.9	349
57	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. *Journal of Chemical Physics*, **2006**, 124, 94108	3.9	108
56	Proper gaussian basis sets for density functional studies of water dimers and trimers. *Journal of Physical Chemistry B*, **2005**, 109, 21471-5	3.4	34
55	Estimation, computation, and experimental correction of molecular zero-point vibrational energies. *Journal of Physical Chemistry A*, **2005**, 109, 6779-89	2.8	42
54	Binding energy curves from nonempirical density functionals. I. Covalent bonds in closed-shell and radical molecules. *Journal of Physical Chemistry A*, **2005**, 109, 11006-14	2.8	53
53	Binding energy curves from nonempirical density functionals II. van der Waals bonds in rare-gas and alkaline-earth diatomics. *Journal of Physical Chemistry A*, **2005**, 109, 11015-21	2.8	79
52	Prescription for the design and selection of density functional approximations: more constraint satisfaction with fewer fits. *Journal of Chemical Physics*, **2005**, 123, 62201	3.9	658
51	Fluorinated cellobiose and maltose as stand-ins for energy surface calculations. *Tetrahedron: Asymmetry*, **2005**, 16, 577-586		21
50	Energies of organic molecules and atoms in density functional theory. *International Journal of Quantum Chemistry*, **2005**, 101, 506-511	2.1	62

49	Implicit Zero-Point Vibration Energy and Thermal Corrections in Rapid Estimation of Enthalpies of Formation from HartreeBock Total Energy and Partial Charges. *Journal of Physical Chemistry A*, **2003**, 107, 736-744	2.8	9
48	Rapid Estimation of Enthalpies of Formation from HartreeBock Total Energy and Partial Charges for Compounds Containing Si, S, and Cl Atoms. *Journal of Physical Chemistry A*, **2003**, 107, 8687-8695	2.8	3
47	Rapid Estimation of Zero-Point Energies of Molecules Using HartreeBock Atomic Partial Charges. *Journal of Physical Chemistry A*, **2003**, 107, 1833-1839	2.8	11
46	Ab initio conformational space study of model compounds of O-glycosides of serine diamide. *Chemistry - A European Journal*, **2002**, 8, 4718-33	4.8	15
45	Proper basis set for quantum mechanical studies of potential energy surfaces of carbohydrates. *Computational and Theoretical Chemistry*, **2002**, 584, 1-4		87
44	Organizing atomic partial charges into a database. *Computational and Theoretical Chemistry*, **2002**, 589-590, 1-5		1
43	Optimal Selection of Partial Charge Calculation Method for Rapid Estimation of Enthalpies of Formation from HartreeBock Total Energy. *Journal of Physical Chemistry A*, **2002**, 106, 12139-12150	2.8	12
42	Accurate thermochemistry from corrected HartreeBock results: rapid estimation of nearly experimental quality total energy using the small 6-31G(d) basis set. *Theoretical Chemistry Accounts* , **2001**, 106, 319-328	1.9	16
41	The performance of the rapid estimation of basis set error and correlation energy from partial charges method on new molecules of the G3/99 test set. *Theoretical Chemistry Accounts*, **2001**, 106, 404-411	1.9	12
40	Fitting atomic correlation parameters for RECEP (rapid estimation of correlation energy from partial charges) method to estimate molecular correlation energies within chemical accuracy. *Journal of Computational Chemistry*, **2001**, 22, 241-254	3.5	18
39	Reproducing Gaussian-3 Total Energy Using Fitted Atomic Correlation Parameters for the Rapid Estimation of Correlation Energy from Partial Charges Method and HartreeBock Results. *Journal of Physical Chemistry A*, **2001**, 105, 1926-1933	2.8	15
38	Prospects in computational molecular medicine: a millennial mega-project on peptide folding. *Computational and Theoretical Chemistry*, **2000**, 500, 5-58		26
37	Ab Initio Conformational Study of Two Lewis X Analogues. *Journal of Physical Chemistry A*, **2000**, 104, 7113-7122	2.8	10
36	Ab Initio Study of Lowest-Energy Conformers of Lewis X (Lex) Trisaccharide. *Journal of Physical Chemistry A*, **2000**, 104, 3381-3390	2.8	17
35	New development in RECEP (rapid estimation of correlation energy from partial charges) method. *Chemical Physics Letters*, **1999**, 307, 469-478	2.5	18
34	Comparison of ab initio and density functional methods for vibrational analysis of TeCl4. *Journal of Computational Chemistry*, **1998**, 19, 308-318	3.5	9
33	Inclusion of exact exchange for self-interaction corrected H3 density functional potential energy surface. *Theoretical Chemistry Accounts*, **1998**, 99, 158-165	1.9	59
32	Theoretical Study of Alternative Ring Forms of β-Fucopyranose. *Journal of Physical Chemistry A*, **1998**, 102, 1219-1229	2.8	26

31	Relative Stability and Structure of Dihydro-1,2,4-triazines: A Theoretical Study. *Journal of Organic Chemistry*, **1998**, 63, 5824-5830	4.2	5
30	The conformational space of selected aldo-pyrano-hexoses. *Computational and Theoretical Chemistry*, **1997**, 395-396, 29-40		26
29	Peptide models XV. The effect of basis set size increase and electron correlation on selected minima of the ab initio 2D-Ramachandran map of For-Gly-NH2 and For-l-Ala-NH2. *Computational and Theoretical Chemistry*, **1997**, 391, 15-26		58
28	The origin of the problems with the PM3 core repulsion function. *Computational and Theoretical Chemistry*, **1997**, 393, 31-38		80
27	Monte Carlo simulation of amorphous systems with the fragment self-consistent field method. *Computational and Theoretical Chemistry*, **1997**, 398-399, 129-133		3
26	Flexible ab initio geometry of methylamine and its internal rotation. *Journal of Molecular Structure*, **1997**, 410-411, 387-390	3.4	1
25	Ab initio and density functional study of the conformational space of 1C4 L-fucose. *Journal of Computational Chemistry*, **1997**, 18, 330-342	3.5	37
24	Simple tests for density functional methods. *Journal of Computational Chemistry*, **1997**, 18, 1534-1545	3.5	22
23	Vibrational analysis of TeCl4. II. A HartreeFock, MP2, and density functional study. *International Journal of Quantum Chemistry*, **1997**, 65, 817-826	2.1	5
22	Prediction of geometrical parameters for silatranes: an ab initio molecular orbital and density functional theory study. *Computational and Theoretical Chemistry*, **1996**, 362, 199-208		24
21	Vibrational properties of C20 isomers, a semi-empirical study. *Journal of Molecular Structure*, **1996**, 376, 513-523	3.4	10
20	The structure of 1-chlorosilatrane: An ab initio molecular orbital and a density functional theory study. *Journal of Computational Chemistry*, **1996**, 17, 767-780	3.5	21
19	Theoretical study of intramolecular hydrogen bonding and molecular geometry of 2-trifluoromethylphenol. *Journal of Computational Chemistry*, **1996**, 17, 1804-1819	3.5	19
18	Relative stability of 1C4 and 4C1 chair forms of D-glucose: a density functional study. *Chemical Physics Letters*, **1996**, 257, 49-60	2.5	78
17	The photoelectron spectrum and conformation of phenylphosphine and phenylarsine. *Structural Chemistry*, **1995**, 6, 1-7	1.8	19
16	The failure of the MO-based theoretical explanations for bending of disiloxane. *Computational and Theoretical Chemistry*, **1995**, 332, 187-188		4
15	Density functional and post Hartree-Fock equilibrium geometries, potential energy surface and vibrational frequencies for methylamine. *Chemical Physics Letters*, **1995**, 233, 611-618	2.5	17
14	Density functional conformational analysis of 1,2-ethanediol. *Chemical Physics Letters*, **1995**, 243, 419-428	2.5	45

13	Ab initio and DFT investigations of intramolecular hydrogen bonding in 1,2-ethanediol. *Chemical Physics Letters*, **1995**, 245, 129-135	2.5	26
12	Density functional study of the equilibrium geometry and Si-O-Si potential energy curve of disiloxane. *Chemical Physics Letters*, **1994**, 229, 191-197	2.5	27
11	Ab initio molecular orbital study of 1-fluorosilatrane. *Journal of Computational Chemistry*, **1994**, 15, 385-394	3.4	25
10	Structure of disiloxane: A semiempirical and Post-Hartree-Fock study. *Journal of Computational Chemistry*, **1994**, 15, 925-936	3.5	21
9	Analysis of the core-repulsion functions used in AM1 and PM3 semiempirical calculations: Conformational analysis of ring systems. *Journal of Computational Chemistry*, **1993**, 14, 895-898	3.5	45
8	Wavenumbers and intensities of the fundamental vibrational modes of HNSi and DNSi from quantum-chemical computations. *Journal of Molecular Structure*, **1993**, 297, 243-253	3.4	1
7	AM1 and PM3 semiempirical molecular orbital study of silatranes III. 1-Chlorosilatrane. *Journal of Organometallic Chemistry*, **1993**, 454, 15-23	2.3	20
6	MNDO, AM1 and PM3 semiempirical molecular orbital study of 1-fluorosilatrane. *Journal of Organometallic Chemistry*, **1993**, 446, 99-106	2.3	21
5	Investigation of heterocyclic compounds containing a P?C or As?C bond by ultraviolet photoelectron spectroscopy. *Journal of Organometallic Chemistry*, **1989**, 373, 49-55	2.3	49
4	Recent advances in fuzzy peak tracking in high-performance liquid chromatography. *Journal of Chromatography A*, **1989**, 485, 557-567	4.5	7
3	Investigation of 3-substituted benzazaphospholes and benzazarsoles by UV-photoelectron spectroscopy. *Journal of Organometallic Chemistry*, **1989**, 373, 57-61	2.3	21
2	The molecular structure of 1-phenylsilatranone. *Journal of Organometallic Chemistry*, **1987**, 329, 305-311	2.3	9
1	1,3-Dipolare cycloadditionen von 6,7-dialkoxy-3,4-dihydroisochinolinium-Salzen. *Tetrahedron*, **1984**, 40, 369-375	2.4	22