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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.

131 papers	9,098 citations	46 h-index	93 g-index
133 ext. papers	9,775 ext. citations	3.6 avg, IF	5.99 L-index

#	Paper	IF	Citations
131	Assessment of a range-separated orbital-optimised random-phase approximation electron correlation method. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	6
130	Performance of Cu -, Pb -, and Hg -Exchanged Mordenite in the Adsorption of I , ICH , H O, CO, ClCH , and Cl : A Density Functional Study. *ChemPhysChem*, **2017**, 18, 1642-1652	3.2	19
129	Casimir-Polder Size Consistency: A Constraint Violated by Some Dispersion Theories. *Journal of Chemical Theory and Computation*, **2017**, 13, 5829-5833	6.4	6
128	A Fractionally Ionic Approach to Polarizability and van der Waals Many-Body Dispersion Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 5920-5930	6.4	62
127	Dielectric Matrix Formulation of Correlation Energies in the Random Phase Approximation: Inclusion of Exchange Effects. *Journal of Chemical Theory and Computation*, **2016**, 12, 2191-202	6.4	27
126	Many-body dispersion corrections for periodic systems: an efficient reciprocal space implementation. *Journal of Physics Condensed Matter*, **2016**, 28, 045201	1.8	69
125	Spooky correlations and unusual van der Waals forces between gapless and near-gapless molecules. *Journal of Chemical Physics*, **2016**, 145, 204107	3.9	2
124	Blind test of density-functional-based methods on intermolecular interaction energies. *Journal of Chemical Physics*, **2016**, 145, 124105	3.9	76
123	Improving the accuracy of ground-state correlation energies within a plane-wave basis set: The electron-hole exchange kernel. *Journal of Chemical Physics*, **2016**, 145, 104105	3.9	15
122	Spin-unrestricted random-phase approximation with range separation: Benchmark on atomization energies and reaction barrier heights. *Journal of Chemical Physics*, **2015**, 142, 154123	3.9	33
121	Relationships between charge density response functions, exchange holes and localized orbitals. *Computational and Theoretical Chemistry*, **2015**, 1053, 44-52	2	4
120	Local random phase approximation with projected oscillator orbitals. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	2
119	Extending the applicability of the Tkatchenko-Scheffler dispersion correction via iterative Hirshfeld partitioning. *Journal of Chemical Physics*, **2014**, 141, 034114	3.9	134
118	Analytical Energy Gradients in Range-Separated Hybrid Density Functional Theory with Random Phase Approximation. *Journal of Chemical Theory and Computation*, **2014**, 10, 1968-79	6.4	19
117	The Black Polymorph of TTF-CA: TTF Polymorphism and Solvent Effects in Mechanochemical and Vapor Digestion Syntheses, FT-IR, Crystal Packing, and Electronic Structure. *Crystal Growth and Design*, **2014**, 14, 91-100	3.5	20
116	Improved Density Dependent Correction for the Description of London Dispersion Forces. *Journal of Chemical Theory and Computation*, **2013**, 9, 4293-9	6.4	138
115	Assessment of range-separated time-dependent density-functional theory for calculating C6 dispersion coefficients. *Journal of Chemical Physics*, **2013**, 138, 194106	3.9	17

114	Chalcogen Bonding: Experimental and Theoretical Determinations from Electron Density Analysis. Geometrical Preferences Driven by Electrophilic/Nucleophilic Interactions. *Crystal Growth and Design*, **2013**, 13, 3283-3289	3.5	134
113	Charge Density Analysis and Topological Properties of Hal3-Synthons and Their Comparison with Competing Hydrogen Bonds. *Crystal Growth and Design*, **2012**, 12, 5373-5386	3.5	65
112	Spin crossover transition of Fe(phen)2(NCS)2: periodic dispersion-corrected density-functional study. *Physical Chemistry Chemical Physics*, **2012**, 14, 5389-96	3.6	51
111	Short range DFT combined with long-range local RPA within a range-separated hybrid DFT framework. *Chemical Physics Letters*, **2012**, 550, 162-169	2.5	28
110	Ab initio study of structure and interconversion of native cellulose phases. *Journal of Physical Chemistry A*, **2011**, 115, 10097-105	2.8	38
109	Periodic projector augmented wave density functional calculations on the hexachlorobenzene crystal and comparison with the experimental multipolar charge density model. *Journal of Physical Chemistry A*, **2011**, 115, 14484-94	2.8	37
108	Intermolecular Interaction Energies from Experimental Charge Density Studies **2011**, 387-433		13
107	Correlation Energy Expressions from the Adiabatic-Connection Fluctuation-Dissipation Theorem Approach. *Journal of Chemical Theory and Computation*, **2011**, 7, 3116-30	6.4	103
106	Linear Response and Measures of Electron Delocalization in Molecules. *Current Organic Chemistry*, **2011**, 15, 3609-3618	1.7	16
105	Monomolecular cracking of propane over acidic chabazite: An ab initio molecular dynamics and transition path sampling study. *Journal of Catalysis*, **2011**, 279, 220-228	7.3	85
104	Aurophilic Interactions from Wave Function, Symmetry-Adapted Perturbation Theory, and Rangehybrid Approaches. *Journal of Chemical Theory and Computation*, **2011**, 7, 2399-407	6.4	34
103	Dispersion interaction in hydrogen-chain models. *Journal of Chemical Physics*, **2011**, 134, 114106	3.9	24
102	Closed-shell ring coupled cluster doubles theory with range separation applied on weak intermolecular interactions. *Journal of Chemical Physics*, **2011**, 135, 084119	3.9	81
101	Cohesive properties and asymptotics of the dispersion interaction in graphite by the random phase approximation. *Physical Review Letters*, **2010**, 105, 196401	7.4	298
100	Range-separated density-functional theory with random phase approximation applied to noncovalent intermolecular interactions. *Journal of Chemical Physics*, **2010**, 132, 244108	3.9	113
99	Improved description of the structure of molecular and layered crystals: ab initio DFT calculations with van der Waals corrections. *Journal of Physical Chemistry A*, **2010**, 114, 11814-24	2.8	737
98	On the equivalence of ring-coupled cluster and adiabatic connection fluctuation-dissipation theorem random phase approximation correlation energy expressions. *Journal of Chemical Physics*, **2010**, 133, 154106	3.9	67
97	Range-separated density-functional theory with the random-phase approximation: Detailed formalism and illustrative applications. *Physical Review A*, **2010**, 82,	2.6	103

96	Adiabatic-connection fluctuation-dissipation density-functional theory based on range separation. *Physical Review Letters*, **2009**, 102, 096404	7.4	222
95	Wigner (2n + 1) rule for nonlinear Schr inger equations. *Journal of Mathematical Chemistry*, **2009**, 46, 1-14	2.1	11
94	Charge density reconstitution from approximate exchange-correlation holes. *Canadian Journal of Chemistry*, **2009**, 87, 1444-1450	0.9	14
93	Assessing the performance of recent density functionals for bulk solids. *Physical Review B*, **2009**, 79,	3.3	530
92	Rayleigh-Schr inger many-body perturbation theory for density functionals: A unified treatment of one- and two-electron perturbations. *Physical Review A*, **2008**, 78,	2.6	22
91	Modeling spin-crossover compounds by periodic DFT+U approach. *Physical Review B*, **2008**, 78,	3.3	67
90	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. *Journal of Chemical Theory and Computation*, **2007**, 3, 1901-13	6.4	35
89	Modeling Induction Phenomena in Intermolecular Interactions with an Ab Initio Force Field. *Journal of Chemical Theory and Computation*, **2007**, 3, 1914-26	6.4	33
88	Proton exchange of small hydrocarbons over acidic chabazite: Ab initio study of entropic effects. *Journal of Catalysis*, **2007**, 250, 171-183	7.3	48
87	On the exchange-hole model of London dispersion forces. *Journal of Chemical Physics*, **2007**, 127, 024108	3.9	49
86	Range separated hybrid density functional with long-range Hartree-Fock exchange applied to solids. *Journal of Chemical Physics*, **2007**, 127, 054101	3.9	86
85	Spherical harmonic expansion of short-range screened Coulomb interactions. *Journal of Physics A*, **2006**, 39, 8613-8630		12
84	Screened hybrid density functionals applied to solids. *Journal of Chemical Physics*, **2006**, 124, 154709	3.9	1591
83	Continuing challenges in the parametrization of intermolecular force fields. Towards an accurate description of electrostatic and induction terms. *New Journal of Chemistry*, **2005**, 29, 411-420	3.6	18
82	van der Waals forces in density functional theory: Perturbational long-range electron-interaction corrections. *Physical Review A*, **2005**, 72,	2.6	265
81	Hybrid functional with separated range. *Chemical Physics Letters*, **2005**, 415, 100-105	2.5	227
80	Potential curves for alkaline-earth dimers by density functional theory with long-range correlation corrections. *Chemical Physics Letters*, **2005**, 416, 370-375	2.5	51
79	Geometry optimization of periodic systems using internal coordinates. *Journal of Chemical Physics*, **2005**, 122, 124508	3.9	106

78	OPEP: a tool for the optimal partitioning of electric properties. *Journal of Computational Chemistry*, **2003**, 24, 997-1008	3.5	37
77	Theoretical CD spectrum calculations of the crown-ether aralkyl-ammonium salt complex. *Chirality*, **2002**, 14, 377-85	2.1	10
76	Approximate electrostatic interaction operator for QM/MM calculations. *Chemical Physics Letters*, **2002**, 356, 331-339	2.5	79
75	Intra- and intermolecular interactions in crystals of polar molecules. A study by the mixed quantum mechanical/molecular mechanical SCMP-NDDO method. *Journal of Computational Chemistry*, **2001**, 22, 1679-1690	3.5	11
74	Fast and accurate determination of induction energies: reduction of topologically distributed polarizability models. *Chemical Physics Letters*, **2001**, 338, 180-188	2.5	30
73	An efficient method for the coordinate transformation problem of massively three-dimensional networks. *Journal of Chemical Physics*, **2001**, 114, 9747-9753	3.9	17
72	Alternative Approaches for the Calculation of Induction Energies: Characterization, Effectiveness, and Pitfalls. *Journal of Physical Chemistry A*, **2001**, 105, 11505-11514	2.8	23
71	Distributed polarizability of the water dimer: Field-induced charge transfer along the hydrogen bond. *Journal of Chemical Physics*, **2001**, 114, 7951-7961	3.9	67
70	Ab Initio Simulations of Zeolite Reactivity. *Progress in Theoretical Chemistry and Physics*, **2001**, 77-108	0.6	3
69	Crystal and electronic structure of two polymorphic modifications of famotidine. An experimental and theoretical study. *Computational and Theoretical Chemistry*, **2000**, 503, 73-79		30
68	Correlation of bond orders and softnesses. *Computational and Theoretical Chemistry*, **2000**, 501-502, 379-388		8
67	Chemical building blocks in quantum chemical calculations. Perspective on the density matrix in many-electron quantum mechanics I. Generalized product functions. Factorization and physical interpretation of the density matrices *Theoretical Chemistry Accounts*, **2000**, 103, 238-241	1.9	7
66	Linear scaling algorithm for the coordinate transformation problem of molecular geometry optimization. *Journal of Chemical Physics*, **2000**, 113, 5598-5603	3.9	26
65	Distributed polarizabilities derived from induction energies: A finite perturbation approach. *Journal of Chemical Physics*, **2000**, 112, 2709-2717	3.9	38
64	Distributed first and second order hyperpolarizabilities: An improved calculation of nonlinear optical susceptibilities of molecular crystals. *Journal of Chemical Physics*, **2000**, 112, 6161-6172	3.9	51
63	Comparison of ab Initio Hartree Fock and Kohn Sham Orbitals in the Calculation of Atomic Charge, Bond Index, and Valence. *Journal of Physical Chemistry A*, **2000**, 104, 9953-9963	2.8	83
62	Determination of Distributed Polarizabilities from a Statistical Analysis of Induction Energies. *Journal of Physical Chemistry A*, **2000**, 104, 1293-1303	2.8	20
61	Covalent bond orders and atomic valences from correlated wavefunctions. *Chemical Physics Letters*, **1999**, 299, 1-8	2.5	53

60	Colour Polymorphism of a Bis(quinoxaline) Compound. *European Journal of Organic Chemistry*, **1999**, 1999, 2119-2125	3.2	13
59	Polymorphism in silica studied in the local density and generalized-gradient approximations. *Journal of Physics Condensed Matter*, **1999**, 11, 3833-3874	1.8	157
58	Statistical analysis of distributed multipoles derived from molecular electrostatic potentials. *Molecular Physics*, **1998**, 94, 881-895	1.7	31
57	On the Nature of Water Interacting with Br□sted Acidic Sites. Ab Initio Molecular Dynamics Study of Hydrated HSAPO-34. *Journal of Physical Chemistry B*, **1998**, 102, 7307-7310	3.4	50
56	Br□sted Acid Sites in HSAPO-34 and Chabazite: An Ab Initio Structural Study. *Journal of Physical Chemistry B*, **1998**, 102, 5573-5580	3.4	146
55	Comment on □New strategies to incorporate the solvent polarization in self-consistent reaction field and free-energy perturbation simulations□[J. Chem. Phys. 103, 10183 (1995)]. *Journal of Chemical Physics*, **1997**, 107, 1291-1292	3.9	14
54	Effect of Polarizability on the Potential of Mean Force of Two Cations. The Guanidinium□Guanidinium Ion Pair in Water. *Journal of Physical Chemistry B*, **1997**, 101, 10910-10917	3.4	70
53	Intermolecular interaction energies by topologically partitioned electric properties II. Dispersion energies in one-centre and multicentre multipole expansions. *Molecular Physics*, **1997**, 91, 145-160	1.7	43
52	The origin of the problems with the PM3 core repulsion function. *Computational and Theoretical Chemistry*, **1997**, 393, 31-38		80
51	Topologically partitioned dynamic polarizabilities using the theory of atoms in molecules. *Canadian Journal of Chemistry*, **1996**, 74, 976-987	0.9	23
50	Mixed quantum□classical calculations on the water molecule in liquid phase: Influence of a polarizable environment on electronic properties. *International Journal of Quantum Chemistry*, **1996**, 58, 251-265	2.1	21
49	Transferability of topologically partitioned polarizabilities: the case of n-alkanes. *Molecular Physics*, **1996**, 89, 595-605	1.7	27
48	Intermolecular interaction energies by topologically partitioned electric properties. 1. Electrostatic and induction energies in one-centre and multicentre multipole expansions. *Molecular Physics*, **1996**, 88, 69-92	1.7	32
47	Choosing between alternative MP2 algorithms in the self-consistent reaction field theory of solvent effects. *Chemical Physics Letters*, **1995**, 241, 51-56	2.5	71
46	Ab initio and DFT investigations of intramolecular hydrogen bonding in 1,2-ethanediol. *Chemical Physics Letters*, **1995**, 245, 129-135	2.5	26
45	A comprehensive approach to molecular charge density models: From distributed multipoles to fitted atomic charges. *International Journal of Quantum Chemistry*, **1994**, 52, 17-37	2.1	45
44	The reliability of the point charge model representing intermolecular effects in ab initio calculations. *Chemical Physics Letters*, **1994**, 225, 258-264	2.5	19
43	Distributed polarizabilities using the topological theory of atoms in molecules. *Chemical Physics Letters*, **1994**, 219, 267-273	2.5	136

42	OSIPE a tool for scientific programming in FORTRAN. *Computer Physics Communications*, **1994**, 81, 293-317	4.2	14
41	Covalent Bond Orders and Atomic Valence Indices in the Topological Theory of Atoms in Molecules. *The Journal of Physical Chemistry*, **1994**, 98, 5244-5248		269
40	Transferable net atomic charges from a distributed multipole analysis for the description of electrostatic properties: a case study of saturated hydrocarbons. *The Journal of Physical Chemistry*, **1993**, 97, 6628-6636		67
39	Modeling amino acid side chains. 2. Determination of point charges from electrostatic properties: toward transferable point charge models. *The Journal of Physical Chemistry*, **1993**, 97, 9788-9796		28
38	Modeling amino acid side chains. 3. Influence of intra- and intermolecular environment on point charges. *The Journal of Physical Chemistry*, **1993**, 97, 9797-9807		18
37	Ab initio determination of electronic energy splitting and transition rates for imidogen in argon matrixes. *The Journal of Physical Chemistry*, **1993**, 97, 10011-10020		6
36	Reaction field factors for a multipole distribution in a cavity surrounded by a continuum. *Chemical Physics Letters*, **1993**, 202, 18-22	2.5	78
35	RayleighSchrdinger perturbation theory for nonlinear Schrdinger equations with linear perturbation. *International Journal of Quantum Chemistry*, **1993**, 47, 469-483	2.1	34
34	Common theoretical framework for quantum chemical solvent effect theories. *Journal of Mathematical Chemistry*, **1992**, 10, 93-137	2.1	63
33	Protein electrostatics on personal computers. *Computational and Theoretical Chemistry*, **1992**, 256, 113-123		5
32	Critical analysis of electric field modeling: Formamide. *Journal of Computational Chemistry*, **1992**, 13, 1234-1245	3.5	28
31	The role of induction forces in infra-red matrix shifts: quantum chemical calculations with reaction field model hamiltonian. *Computational and Theoretical Chemistry*, **1991**, 232, 97-110		5
30	Normalization corrections to perturbation theory for the time-independent nonlinear Schrdinger equation. *Physical Review A*, **1991**, 44, 2188-2191	2.6	12
29	Peptide models. 1. Topology of selected peptide conformational potential energy surfaces (glycine and alanine derivatives). *Journal of the American Chemical Society*, **1991**, 113, 6256-6265	16.4	233
28	Chemical Fragmentation Approach to the Quantum Chemical Description of Extended Systems **1991**, 1-49		6
27	Chemical Fragmentation Approach to the Quantum Chemical Description of Extended Systems **1991**, 1-49		2
26	Quantum-chemical model calculations on the acidic site of zeolites including Madelung-potential effects. *Chemical Physics Letters*, **1990**, 168, 461-467	2.5	48
25	Modelling the electric field of water obtained from accurate SCF wave functions. *Chemical Physics Letters*, **1990**, 172, 55-61	2.5	16

24	Computational chemistry on a PC. *International Journal of Quantum Chemistry*, **1990**, 38, 163-171	2.1	3
23	Are direct reaction field methods appropriate for describing dispersion interactions?. *Chemical Physics Letters*, **1990**, 175, 313-318	2.5	18
22	Analytical first and second energy derivatives in the polarization model. *Chemical Physics Letters*, **1990**, 166, 180-188	2.5	21
21	Calculations on electrostatic properties of HY zeolite. *Journal of the Chemical Society, Faraday Transactions*, **1990**, 86, 3461-3466		8
20	A study on the backbone/side-chain interaction in N-formyl-(L)serineamide. *Canadian Journal of Chemistry*, **1990**, 68, 1882-1888	0.9	19
19	Generalized self-consistent reaction field theory in a multicenter-multipole ab-initio LCGO framework. I. Electronic properties of the water molecule in a Monte Carlo sample of liquid water molecules studied with standard basis sets. *Journal De Chimie Physique Et De Physico-Chimie Biologique*, **1990**, 87, 875-903		34
18	Intramolecular sulfur-oxygen interaction in sulfonium compounds and sulfoxides. *Computational and Theoretical Chemistry*, **1989**, 186, 53-60		4
17	Bond orders in three-centre bonds. *Computational and Theoretical Chemistry*, **1989**, 186, 61-67		12
16	Calculation of electrostatic potentials and fields inside zeolite cavities. *Collection of Czechoslovak Chemical Communications*, **1988**, 53, 2308-2319		9
15	The use of theoretical indices for the characterization of S?O linkage multiplicity. *Computational and Theoretical Chemistry*, **1988**, 165, 273-287		17
14	Electrostatic interactions in three-dimensional solids. Self-consistent Madelung potential (SCMP) approach. *Journal of Chemical Physics*, **1987**, 86, 6957-6966	3.9	36
13	Electrostatic complementarity in molecular aggregates. *Computational and Theoretical Chemistry*, **1987**, 149, 169-176		6
12	Bonding between nonbonded sulfur and oxygen atoms in selected organic molecules (a quantum chemical study). *Journal of the American Chemical Society*, **1987**, 109, 2237-2245	16.4	109
11	Molecular electrostatic fields from bond fragments. *International Journal of Quantum Chemistry*, **1987**, 31, 927-939	2.1	36
10	Surface modification by substitution. *Chemical Physics Letters*, **1987**, 136, 1-8	2.5	13
9	The role of optimum supplementary d-orbitals for hypervalent selenium compounds. *Chemical Physics Letters*, **1986**, 131, 247-251	2.5	6
8	Ab initio quantum chemical study of the structure and vibrational spectra of the vinylene carbonate molecule. *The Journal of Physical Chemistry*, **1986**, 90, 6420-6424		2
7	Noncovalent structural models for the Asp-His dyad in the active site of serine proteases and for solid-state switching of protonation states: crystal structure of the associates of 1,1'-binaphthyl-2,2'-dicarboxylic acid with imidazole in dihydrated and in anhydrous forms. *Journal of the American Chemical Society*, **1986**, 108, 1275-1281	16.4	22

6	Structure and ring inversion of 2-pyrrolidone. Semiempirical quantum chemical study and analysis of X-ray data. *Collection of Czechoslovak Chemical Communications*, **1986**, 51, 249-263		3
5	Intramolecular sulfur□oxygen interaction: An ab initio conformational study of (Z)-3-fluorothio-2-propenal. *Computational and Theoretical Chemistry*, **1985**, 123, 189-201		22
4	Synthesis of Vinca alkaloids and related compounds. Part 18. Stereochemical investigations on some intermediates leading to (+)-vincamine. *Journal of the Chemical Society Perkin Transactions II*, **1984**, 1629-1636		3
3	Comparison of protein electrostatic potential along the catalytic triad of serine proteinases. *Journal of Theoretical Biology*, **1983**, 103, 349-56	2.3	35
2	Perturbation theory for nonlinear time-independent Schr□dinger equations. *Physical Review A*, **1983**, 28, 45-48	2.6	30
1	A SCRF-CNDO/2 study on proton conductivity mechanisms in hydronium perchlorate. Towards a quantum chemical representation of defects and impurities in crystals. *Journal of Chemical Physics*, **1982**, 77, 4723-4733	3.9	32