Evert Jan Baerends

List of Publications by Year
in descending order

425 papers	67,961 citations	1535 106 h-index	735 251 g-index
445 all docs	445 docs citations	445 times ranked	24059 citing authors

#	Article	IF	Citations
1	Chemistry with ADF. Journal of Computational Chemistry, 2001, 22, 931-967.	3.3	8,854
2	Relativistic regular twoâ€component Hamiltonians. Journal of Chemical Physics, 1993, 99, 4597-4610.	3.0	3,800
3	Self-consistent molecular Hartreeâ€"Fockâ€"Slater calculations I. The computational procedure. Chemical Physics, 1973, 2, 41-51.	1.9	3,106
4	Relativistic total energy using regular approximations. Journal of Chemical Physics, 1994, 101, 9783-9792.	3.0	2,823
5	Towards an order-. Theoretical Chemistry Accounts, 1998, 99, 391.	1.4	2,434
6	Optimized Slater-type basis sets for the elements 1-118. Journal of Computational Chemistry, 2003, 24, 1142-1156.	3.3	2,314
7	Geometry optimizations in the zero order regular approximation for relativistic effects. Journal of Chemical Physics, 1999, 110, 8943-8953.	3.0	2,170
8	The zeroâ€order regular approximation for relativistic effects: The effect of spinâ€"orbit coupling in closed shell molecules. Journal of Chemical Physics, 1996, 105, 6505-6516.	3.0	1,465
9	Exchange-correlation potential with correct asymptotic behavior. Physical Review A, 1994, 49, 2421-2431.	2.5	1,343
10	Towards an order- N DFT method. Theoretical Chemistry Accounts, 1998, 99, 391-403.	1.4	1,283
11	Relativistic regular two-component Hamiltonians. International Journal of Quantum Chemistry, 1996, 57, 281-293.	2.0	1,039
12	Voronoi deformation density (VDD) charges: Assessment of the Mulliken, Bader, Hirshfeld, Weinhold, and VDD methods for charge analysis. Journal of Computational Chemistry, 2004, 25, 189-210.	3.3	956
13	On the calculation of multiplet energies by the hartree-fock-slater method. Theoretica Chimica Acta, 1977, 43, 261-271.	0.8	912
14	Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry. Reviews in Computational Chemistry, 2007, , 1-86.	1.5	775
15	Three-dimensional numerical integration for electronic structure calculations. International Journal of Quantum Chemistry, 1988, 33, 87-113.	2.0	740
16	Molecular calculations of excitation energies and (hyper)polarizabilities with a statistical average of orbital model exchange-correlation potentials. Journal of Chemical Physics, 2000, 112, 1344-1352.	3.0	699
17	Implementation of time-dependent density functional response equations. Computer Physics Communications, 1999, 118, 119-138.	7.5	613
18	A Quantum Chemical View of Density Functional Theory. Journal of Physical Chemistry A, 1997, 101, 5383-5403.	2.5	576

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19	Electronic structure, magnetic properties, ESR, and optical spectra for 2-iron ferredoxin models by LCAO-X.alpha. valence bond theory. Journal of the American Chemical Society, 1984, 106, 2316-2327.	13.7	517
20	Assessment of Conventional Density Functional Schemes for Computing the Dipole Moment and (Hyper)polarizabilities of Pushâ^'Pull Ï€-Conjugated Systemsâ€. Journal of Physical Chemistry A, 2000, 104, 4755-4763.	2.5	501
21	Interpretation of the Kohnâ€“Sham orbital energies as approximate vertical ionization potentials. Journal of Chemical Physics, 2002, 116, 1760-1772.	3.0	474
22	Density functional calculations of nuclear magnetic shieldings using the zeroth-order regular approximation (ZORA) for relativistic effects: ZORA nuclear magnetic resonance. Journal of Chemical Physics, 1999, 110, 7689-7698.	3.0	464
23	Precise density-functional method for periodic structures. Physical Review B, 1991, 44, 7888-7903.	3.2	453
24	Assessment of conventional density functional schemes for computing the polarizabilities and hyperpolarizabilities of conjugated oligomers: An ab initio investigation of polyacetylene chains. Journal of Chemical Physics, 1998, 109, 10489-10498.	3.0	453
25	Self-consistent molecular Hartreeâ€"Fockâ€"Slater calculations II. The effect of exchange scaling in some small molecules. Chemical Physics, 1973, 2, 52-59.	1.9	420
26	Hydrogen Bonding in DNA Base Pairs:â€‰ Reconciliation of Theory and Experiment. Journal of the American Chemical Society, 2000, 122, 4117-4128.	13.7	418
27	Approximation of the exchange-correlation Kohnâ€“Sham potential with a statistical average of different orbital model potentials. Chemical Physics Letters, 1999, 302, 199-207.	2.6	409
28	Chiroptical properties from time-dependent density functional theory. I. Circular dichroism spectra of organic molecules. Journal of Chemical Physics, 2002, 116, 6930-6940.	3.0	386
29	Binding energy and electronic structure of small copper particles. Physical Review B, 1983, 27, 2132-2144.	3.2	385
30	Calculation of bond energies in compounds of heavy elements by a quasi-relativistic approach. The Journal of Physical Chemistry, 1989, 93, 3050-3056.	2.9	350
31	The Kohnâ€“Sham gap, the fundamental gap and the optical gap: the physical meaning of occupied and virtual Kohnâ€“Sham orbital energies. Physical Chemistry Chemical Physics, 2013, 15, 16408.	2.8	349
32	Shape corrections to exchange-correlation potentials by gradient-regulated seamless connection of model potentials for inner and outer region. Journal of Chemical Physics, 2001, 114, 652.	3.0	343
33	The Nature of the Hydrogen Bond in DNA Base Pairs: The Role of Charge Transfer and Resonance Assistance. Chemistry - A European Journal, 1999, 5, 3581-3594.	3.3	340
34	Electric Field Dependence of the Exchange-Correlation Potential in Molecular Chains. Physical Review Letters, 1999, 83, 694-697.	7.8	339
35	A perturbation theory approach to relativistic calculations. Molecular Physics, 1979, 38, 1909-1929.	1.7	334
36	Electronic Spectra of M(CO)6(M = Cr, Mo, W) Revisited by a Relativistic TDDFT Approach. Journal of the American Chemical Society, 1999, 121, 10356-10365.	13.7	330

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37	Asymptotic correction of the exchangeâ€“correlation kernel of time-dependent density functional theory for long-range charge-transfer excitations. Journal of Chemical Physics, 2004, 121, 655-660.	3.0	327
38	A density functional theory study of frequencyâ€dependent polarizabilities and Van der Waals dispersion coefficients for polyatomic molecules. Journal of Chemical Physics, 1995, 103, 9347-9354.	3.0	313
39	A DFT/TDDFT interpretation of the ground and excited states of porphyrin and porphyrazine complexes. Coordination Chemistry Reviews, 2002, 230, 5-27.	18.8	290
40	The Carbonâ^'Lithium Electron Pair Bond in (CH3Li)n(n= 1, 2, 4). Organometallics, 1996, 15, 2923-2931.	2.3	286
41	Relativistic effects on bonding. Journal of Chemical Physics, 1981, 74, 1271-1284.	3.0	254
42	Density-functional-theory response-property calculations with accurate exchange-correlation potentials. Physical Review A, 1998, 57, 2556-2571.	2.5	246
43	An approximate exchange-correlation hole density as a functional of the natural orbitals. Molecular Physics, 2002, 100, 401-421.	1.7	245
44	Self-consistent approximation to the Kohn-Sham exchange potential. Physical Review A, 1995, 51, 1944-1954.	2.5	238
45	The calculation of excitation energies based on the relativistic two-component zeroth-order regular approximation and time-dependent density-functional with full use of symmetry. Journal of Chemical Physics, 2005, 122, 204103.	3.0	238
46	Ground State of the (H2O)2+ Radical Cation:â€‰ DFT versus Post-Hartreeâ^'Fock Methods. Journal of Physical Chemistry A, 1999, 103, 166-170.	2.5	232
47	The Case for Steric Repulsion Causing the Staggered Conformation of Ethane. Angewandte Chemie - International Edition, 2003, 42, 4183-4188.	13.8	225
48	Even-tempered slater-type orbitals revisited: From hydrogen to krypton. Journal of Computational Chemistry, 2004, 25, 1030-1036.	3.3	212
49	The merits of the frozen-density embedding scheme to model solvatochromic shifts. Journal of Chemical Physics, 2005, 122, 094115.	3.0	207
50	Cohesive energy of 3dtransition metals: Density functional theory atomic and bulk calculations. Physical Review B, 1996, 54, 5326-5333.	3.2	204
51	Excitation Energies for Transition Metal Compounds from Time-Dependent Density Functional Theory. Applications to MnO4-, Ni(CO)4, and Mn2(CO)10. Journal of Physical Chemistry A, 1999, 103, 6835-6844.	2.5	199
52	Atomic and molecular hydrogen interacting with Pt(111). Journal of Chemical Physics, 1999, 111, 11155-11163.	3.0	197
53	Physical Meaning of Virtual Kohnâ€“Sham Orbitals and Orbital Energies: An Ideal Basis for the Description of Molecular Excitations. Journal of Chemical Theory and Computation, 2014, 10, 4432-4441.	5.3	195
54	Exchange and correlation energy in density functional theory: Comparison of accurate density functional theory quantities with traditional Hartreeâ€“Fock based ones and generalized gradient approximations for the molecules Li2, N2, F2. Journal of Chemical Physics, 1997, 107, 5007-5015.	3.0	194

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55	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	2.6	192
56	Improved density functional theory results for frequencyâ€dependent polarizabilities, by the use of an exchangeâ€correlation potential with correct asymptotic behavior. Journal of Chemical Physics, 1996, 105, 3142-3151.	3.0	191
57	Central bond in the three CN.cntdot.dimers NC-CN, CN-CN and CN-NC: electron pair bonding and Pauli repulsion effects. The Journal of Physical Chemistry, 1992, 96, 4864-4873.	2.9	190
58	Calculating frequency-dependent hyperpolarizabilities using time-dependent density functional theory. Journal of Chemical Physics, 1998, 109, 10644-10656.	3.0	190
59	Chiroptical properties from time-dependent density functional theory. II. Optical rotations of small to medium sized organic molecules. Journal of Chemical Physics, 2002, 117, 581-592.	3.0	186
60	Time-dependent Density Functional Results for the Dynamic Hyperpolarizability ofC60. Physical Review Letters, 1997, 78, 3097-3100.	7.8	185
61	Fenton-like Chemistry in Water:Â Oxidation Catalysis by Fe(III) and H2O2. Journal of Physical Chemistry A, 2003, 107, 5722-5731.	2.5	182
62	Reactive and Nonreactive Scattering of H2 from a Metal Surface Is Electronically Adiabatic. Science, 2006, 312, 86-89.	12.6	180
63	An improved density matrix functional by physically motivated repulsive corrections. Journal of Chemical Physics, 2005, 122, 204102.	3.0	176
64	Alternatives to the CO Ligand: Coordination of the Isolobal Analogues BF, BNH2, BN(CH3)2, and BOâ‹¯ in Mono- and Binuclear First-Row Transition Metal Complexes. Chemistry - A European Journal, 1998, 4, 210-221.	3.3	172
65	A Density Functional Study of the MLCT States of [Ru(bpy)3]2+ in D3 Symmetry. Inorganic Chemistry, 1994, 33, 3538-3543.	4.0	169
66	Time-dependent density functional calculations on the electronic absorption spectrum of free base porphin. Journal of Chemical Physics, 1999, 111, 2499-2506.	3.0	168
67	Accurate density functional calculations on frequency-dependent hyperpolarizabilities of small molecules. Journal of Chemical Physics, 1998, 109, 10657-10668.	3.0	166
68	Quantum Theory of Dissociative Chemisorption on Metal Surfaces. Accounts of Chemical Research, 2002, 35, 193-200.	15.6	165
69	The Mechanism of Zinc(II)-Dithiocarbamate-Accelerated Vulcanization Uncovered; Theoretical and Experimental Evidence. Journal of the American Chemical Society, 1999, 121, 163-168.	13.7	163
70	Can the Counterpoise Correction for Basis Set Superposition Effect Be Justified?. Journal of Chemical Theory and Computation, 2014, 10, 252-267.	5.3	162
71	Relativistic calculations on the adsorption of CO on the (111) surfaces of Ni, Pd, and Pt within the zeroth-order regular approximation. Physical Review B, 1997, 56, 13556-13562.	3.2	161
72	The electronic structure of transition metal carbonyl complexes. Molecular Physics, 1975, 30, 1735-1747.	1.7	156

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73	Orbital structure of the Kohn-Sham exchange potential and exchange kernel and the field-counteracting potential for molecules in an electric field. Physical Review A, 2001, 64, .	2.5	156
74	Analysis of electron interaction and atomic shell structure in terms of local potentials. Journal of Chemical Physics, 1994, 101, 8955-8963.	3.0	154
75	Atomic reference energies for density functional calculations. Chemical Physics Letters, 1997, 265, 481-489.	2.6	154
76	Metal-Macrocycle Interaction in Phthalocyanines: Density Functional Calculations of Ground and Excited States. Inorganic Chemistry, 1994, 33, 584-595.	4.0	153
77	Polyoxometalates with Internal Cavities:â€‰ Redox Activity, Basicity, and Cation Encapsulation in [Xⁿ⁺P₅W₃₀O₁₁₀]⁽¹⁵⁻ⁿ/s Preyssler Complexes, with X = Na⁺, Ca²⁺, Y³⁺, La³⁺, Ce³⁺, and Th⁴⁺. Journal of the American Chemical Society, 2007, 129, 12244-12253.	13.7	152
78	Comparison of the Accurate Kohnâ^'Sham Solution with the Generalized Gradient Approximations (GGAs) for the SN2 Reaction F- + CH3F â†' FCH3 + F-:â€‰ A Qualitative Rule To Predict Success or Failure of GGAs. Journal of Physical Chemistry A, 2000, 104, 8558-8565.	2.5	151
79	Analysis of correlation in terms of exact local potentials: Applications to two-electron systems. Physical Review A, 1989, 40, 4190-4202.	2.5	144
80	Exact solutions of regular approximate relativistic wave equations for hydrogenâ€like atoms. Journal of Chemical Physics, 1994, 101, 1272-1281.	3.0	142
81	Ethylene epoxidation on silver(110): the role of subsurface oxygen. The Journal of Physical Chemistry, 1989, 93, 6469-6475.	2.9	141
82	Self-consistent molecular Hartree-Fock-Slater calculations. Chemical Physics, 1975, 8, 412-418.	1.9	140
83	Relativistic atomic orbital contractions and expansions: magnitudes and explanations. Journal of Physics B: Atomic, Molecular and Optical Physics, 1990, 23, 3225-3240.	1.5	140
84	The ZORA formalism applied to the Dirac-Fock equation. Chemical Physics Letters, 1995, 246, 632-640.	2.6	139
85	Constructing accurate potential energy surfaces for a diatomic molecule interacting with a solid surface: H2+Pt(111) and H2+Cu(100). Journal of Chemical Physics, 2002, 116, 3841-3855.	3.0	136
86	DFT Study of the Active Intermediate in the Fenton Reaction. Chemistry - A European Journal, 2001, 7, 2775-2783.	3.3	135
87	Ground and Excited States of Zinc Phthalocyanine Studied by Density Functional Methods. Journal of Physical Chemistry A, 2001, 105, 5242-5254.	2.5	132
88	Effects of Porphyrin Core Saddling,meso-Phenyl Twisting, and Counterions on the Optical Properties ofmeso-Tetraphenylporphyrin Diacids:Â The [H4TPP](X)2(X = F, Cl, Br, I) Series as a Case Study. Journal of Physical Chemistry A, 2003, 107, 11468-11482.	2.5	131
89	Cluster studies of CO adsorption. III. CO on small Cu clusters. Journal of Chemical Physics, 1983, 78, 5663-5681.	3.0	130
90	An Explicit Quantum Chemical Method for Modeling Large Solvation Shells Applied to Aminocoumarin C151. Journal of Physical Chemistry A, 2005, 109, 7805-7814.	2.5	130

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91	Basis Set Effects in Density Functional Calculations on the Metalâ^'Ligand and Metalâ^'Metal Bonds of Cr(CO)5â^'CO and (CO)5Mnâ^'Mn(CO)5. The Journal of Physical Chemistry, 1996, 100, 5690-5696.	2.9	127
92	The Optical Spectra of NiP, NiPz, NiTBP, and NiPc:Â Electronic Effects ofMeso-tetraaza Substitution and Tetrabenzo Annulation. Journal of Physical Chemistry A, 2001, 105, 3311-3327.	2.5	127
93	Assessment of a simple correction for the long-range charge-transfer problem in time-dependent density-functional theory. Journal of Chemical Physics, 2006, 124, 214102.	3.0	126
94	The electronic structures of tetrahedral oxo-complexes. The nature of the â€œcharge transferâ€• transitions. Chemical Physics, 1976, 16, 209-217.	1.9	124
95	One - determinantal pure state versus ensemble Kohn-Sham solutions in the case of strong electron correlation: CH 2 and C 2. Theoretical Chemistry Accounts, 1998, 99, 329-343.	1.4	123
96	Physical interpretation and evaluation of the Kohnâ€“Sham and Dyson components of the Îµâ€“I relations between the Kohnâ€“Sham orbital energies and the ionization potentials. Journal of Chemical Physics, 2003, 119, 1937-1950.	3.0	122
97	Six-Dimensional Quantum Dynamics of Dissociative Chemisorption of (v=0,j=0)H2on Cu(100). Physical Review Letters, 1997, 78, 3583-3586.	7.8	121
98	Exact Exchange-Correlation Treatment of DissociatedH2in Density Functional Theory. Physical Review Letters, 2001, 87, 133004.	7.8	121
99	An analytical sixâ€dimensional potential energy surface for dissociation of molecular hydrogen on Cu(100). Journal of Chemical Physics, 1996, 104, 7344-7358.	3.0	118
100	Density functional calculations of nuclear quadrupole coupling constants in the zero-order regular approximation for relativistic effects. Journal of Chemical Physics, 2000, 112, 8279-8292.	3.0	118
101	Nucleophilic or Electrophilic Phosphinidene Complexes MLnPH; What Makes the Difference?. Journal of the American Chemical Society, 2002, 124, 2831-2838.	13.7	115
102	On the required shape corrections to the local density and generalized gradient approximations to the Kohnâ€“Sham potentials for molecular response calculations of (hyper)polarizabilities and excitation energies. Journal of Chemical Physics, 2002, 116, 9591-9601.	3.0	113
103	Quadratic integration over the three-dimensional Brillouin zone. Journal of Physics Condensed Matter, 1991, 3, 6721-6742.	1.8	112
104	Reactive and diffractive scattering of H2 from Pt(111) studied using a six-dimensional wave packet method. Journal of Chemical Physics, 2002, 117, 5885-5898.	3.0	111
105	Relativistic DFT Calculations of the Paramagnetic Intermediates of [NiFe] Hydrogenase. Implications for the Enzymatic Mechanism. Journal of the American Chemical Society, 2001, 123, 5839-5840.	13.7	109
106	Ensuring proper short-range and asymptotic behavior of the exchange-correlation Kohn-Sham potential by modeling with a statistical average of different orbital model potentials. International Journal of Quantum Chemistry, 2000, 76, 407-419.	2.0	106
107	Effect of molecular dissociation on the exchange-correlation Kohn-Sham potential. Physical Review A, 1996, 54, 1957-1972.	2.5	105
108	Density functional results for isotropic and anisotropic multipole polarizabilities and C6, C7, and C8 Van der Waals dispersion coefficients for molecules. Journal of Chemical Physics, 1997, 106, 5091-5101.	3.0	105

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109	Analysis of nondynamical correlation in the metalâ€“ligand bond. Pauli repulsion and orbital localization in MnOâ‚4. Journal of Chemical Physics, 1990, 93, 4129-4141.	3.0	104
110	Molecular Kohn-Sham exchange-correlation potential from the correlatedab initioelectron density. Physical Review A, 1995, 52, 1870-1874.	2.5	103
111	Methane-to-Methanol Oxidation by the Hydrated Iron(IV) Oxo Species in Aqueous Solution:Â A Combined DFT and Carâ€Parrinello Molecular Dynamics Study. Journal of the American Chemical Society, 2004, 126, 4355-4365.	13.7	102
112	The Role of Equatorial and Axial Ligands in Promoting the Activity of Non-Heme Oxidoiron(IV) Catalysts in Alkane Hydroxylation. European Journal of Inorganic Chemistry, 2007, 2007, 3023-3033.	2.0	102
113	CO on Pt(111): A puzzle revisited. Journal of Chemical Physics, 2003, 119, 4522-4528.	3.0	101
114	Synthesis and structure of aryl-substituted phospha-alkenes. Tetrahedron, 1984, 40, 765-776.	1.9	99
115	Dissociation Energies, Vibrational Frequencies, and13C NMR Chemical Shifts of the 18-Electron Species [M(CO)6]n(M = Hfâ€lr, Mo, Tc, Ru, Cr, Mn, Fe). A Density Functional Study. Inorganic Chemistry, 1997, 36, 5031-5036.	4.0	99
116	The analog of Koopmansâ€™ theorem in spin-density functional theory. Journal of Chemical Physics, 2002, 117, 9154-9159.	3.0	98
117	A density matrix functional with occupation number driven treatment of dynamical and nondynamical correlation. Journal of Chemical Physics, 2008, 129, 164105.	3.0	98
118	On the origin of relativistic bond contraction. Chemical Physics Letters, 1980, 75, 1-4.	2.6	97
119	Crâ€CO Photodissociation in Cr(CO)6:â€‰ Reassessment of the Role of Ligand-Field Excited States in the Photochemical Dissociation of Metalâ€Ligand Bonds. Journal of the American Chemical Society, 1997, 119, 7324-7329.	13.7	93
120	Exchange potential from the common energy denominator approximation for the Kohnâ€“Sham Greenâ€™s function: Application to (hyper)polarizabilities of molecular chains. Journal of Chemical Physics, 2002, 116, 6435-6442.	3.0	91
121	Excitation energies of dissociating H2: A problematic case for the adiabatic approximation of time-dependent density functional theory. Journal of Chemical Physics, 2000, 113, 8478-8489.	3.0	90
122	MSi2/Si(111) (M=Co,Ni) interface chemical bond. Physical Review Letters, 1988, 60, 1743-1746.	7.8	89
123	The origin of relativistic effects of atomic orbitals. Journal of Physics B: Atomic, Molecular and Optical Physics, 1989, 22, 1515-1529.	1.5	89
124	Activation of the Câ€H Bond by Electrophilic Attack: Theoretical Study of the Reaction Mechanism of the Aerobic Oxidation of Alcohols to Aldehydes by the Cu(bipy)²⁺/2,2,6,6-Tetramethylpiperidinyl-1-oxy Cocatalyst System. Inorganic Chemistry, 2009, 48, 11909-11920.	4.0	89
125	Theoretical investigation on base-induced 1,2-eliminations in the model system fluoride ion + fluoroethane. The role of the base as a catalyst. Journal of the American Chemical Society, 1993, 115, 9160-9173.	13.7	87
126	Solvation Effects on the SN2 Reaction between CH3Cl and Cl-in Water. Journal of Physical Chemistry A, 2001, 105, 3300-3310.	2.5	87

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127	EPR Characteristics of the [(NC)5M(NO)]3-Ions (M = Fe, Ru, Os). Experimental and DFT Study Establishing NOâ€¢as a Ligand. Inorganic Chemistry, 2001, 40, 5704-5707.	4.0	87
128	A vibrational circular dichroism implementation within a Slater-type-orbital based density functional framework and its application to hexa- and hepta-helicenes. Theoretical Chemistry Accounts, 2008, 119, 245-263.	1.4	87
129	Time-dependent density-matrix-functional theory. Physical Review A, 2007, 75, .	2.5	86
130	Perspective on "Self-consistent equations including exchange and correlation effects". Theoretical Chemistry Accounts, 2000, 103, 265-269.	1.4	85
131	Robust normal modes in vibrational circular dichroism spectra. Physical Chemistry Chemical Physics, 2009, 11, 6107.	2.8	85
132	A Carâ€“Parrinello study of the formation of oxidizing intermediates from Fenton's reagent in aqueous solution. Physical Chemistry Chemical Physics, 2002, 4, 3619-3627.	2.8	84
133	The Effect of Microsolvation on E2 and S_N2 Reactions: Theoretical Study of the Model System F^{â^'} + C₂H₅F + nHF. Chemistry - A European Journal, 1996, 2, 196-207.	3.3	83
134	The Failure of Generalized Gradient Approximations (GGAs) and Meta-GGAs for the Two-Center Three-Electron Bonds in He2+, (H2O)2+, and (NH3)2+. Journal of Physical Chemistry A, 2001, 105, 9211-9218.	2.5	83
135	The spin-unrestricted molecular Kohnâ€“Sham solution and the analogue of Koopmansâ€™s theorem for open-shell molecules. Journal of Chemical Physics, 2004, 120, 8364-8372.	3.0	83
136	Slab versus cluster approach for chemisorption studies. CO on Cu (100). Chemical Physics, 1993, 177, 399-406.	1.9	82
137	A relativistic lcao hartree-fock-slater investigation of the electronic structure of the actinocenes M(COT)2, M = Th, Pa, U, Np AND Pu. Chemical Physics, 1988, 122, 357-374.	1.9	81
138	The effect of density-gradient corrections for a molecule-surface potential energy surface. Slab calculations on Cu(100)c(2x2)-CO. Chemical Physics Letters, 1994, 226, 583-588.	2.6	81
139	O2 Evolution in the Fenton Reaction. Chemistry - A European Journal, 2003, 9, 3436-3444.	3.3	81
140	Vibronic coupling and double excitations in linear response time-dependent density functional calculations: Dipole-allowed states of N2. Journal of Chemical Physics, 2004, 121, 6155-6166.	3.0	80
141	Calculation of harmonic frequencies and harmonic force fields by the hartree-fock-slater method. International Journal of Quantum Chemistry, 1988, 34, 173-181.	2.0	79
142	Molecular exchangeâ€•correlation Kohnâ€“Sham potential and energy density from ab initio firstâ€•and secondâ€•order density matrices: Examples for XH (X=Li, B, F). Journal of Chemical Physics, 1996, 104, 8535-8545.	3.0	79
143	Synergism of Porphyrin-Core Saddling and Twisting ofmeso-Aryl Substituents. Journal of Physical Chemistry A, 2006, 110, 5180-5190.	2.5	79
144	An evaluation of the density functional approach in the zero order regular approximation for relativistic effects: Magnetic interactions in small metal compounds. Journal of Chemical Physics, 2001, 114, 4421.	3.0	78

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145	A Theoretical study of the interaction of ethylene with transition metal complexes. Theoretica Chimica Acta, 1972, 27, 339-354.	0.8	77
146	A theoretical study of the linear versus bent geometry for several MX2 molecules: MgF2, CaH2, CaF2, CeO2 and YbCl2. Polyhedron, 1990, 9, 1919-1934.	2.2	75
147	Six-dimensional quantum dynamics of dissociative chemisorption of H2 on Cu(100). Journal of Chemical Physics, 1997, 107, 3309-3323.	3.0	74
148	Benchmark calculations of chemical reactions in density functional theory: Comparison of the accurate Kohnâ€“Sham solution with generalized gradient approximations for the H2+H and H2+H2 reactions. Journal of Chemical Physics, 1999, 111, 4056-4067.	3.0	74
149	A Density Functional Study of the Optical Spectra and Nonlinear Optical Properties of Heteroleptic Tetrapyrrole Sandwich Complexes:Â The Porphyrinatoâ^'Porphyrazinatoâ^'Zirconium(IV) Complex as a Case Study. Journal of Physical Chemistry A, 2000, 104, 635-643.	2.5	74
150	Excitation Energies of Metal Complexes with Time-dependent Density Functional Theory. Structure and Bonding, 2004, , 49-116.	1.0	74
151	Dissociation of H2on Cu(100): Dynamics on a new twoâ€dimensional potential energy surface. Journal of Chemical Physics, 1995, 102, 3873-3883.	3.0	73
152	Effects of Complex Formation on Vibrational Circular Dichroism Spectra. Journal of Physical Chemistry A, 2008, 112, 6978-6991.	2.5	73
153	A theoretical study of metalâ€"ligand bond strengths (Mî—¸L: L = OH, OCH3, SH, NH2, PH2, CH3, SiH3, CN and) Tj ETQq1 1 0.784314 rg LCo(CO)4. Polyhedron, 1988, 7, 1625-1637.	2.2	72
154	Charge Transfer, Double and Bond-Breaking Excitations with Time-Dependent Density Matrix Functional Theory. Physical Review Letters, 2008, 101, 033004.	7.8	72
155	Molecular cluster theory of CO chemisorption on a nickel(100) surface. Surface Science, 1977, 64, 649-667.	1.9	71
156	What Singles out the FeO²⁺Moiety? A Density-Functional Theory Study of the Methane-to-Methanol Reaction Catalyzed by the First Row Transition-Metal Oxide Dications MO(H₂O)_p²⁺, M = Vâ^'Cu. Inorganic Chemistry, 2009, 48, 3628-3638.	4.0	71
157	Relativistic Effects for NMR Shielding Constants in Transition Metal Oxides Using the Zeroth-Order Regular Approximation. Journal of Physical Chemistry A, 2000, 104, 5600-5611.	2.5	70
158	Electronic spectrum of UO22+ and [UO2Cl4]2â^' calculated with time-dependent density functional theory. Journal of Chemical Physics, 2007, 126, 194311.	3.0	70
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