Evert Jan Baerends

List of Publications by Year
in descending order

352 papers	55,869 citations	2062 97 h-index	989 230 g-index
373 all docs	373 docs citations	373 times ranked	20857 citing authors

#	Article	IF	Citations
1	Chemistry with ADF. Journal of Computational Chemistry, 2001, 22, 931-967.	3.4	9,113
2	Relativistic regular twoâ€component Hamiltonians. Journal of Chemical Physics, 1993, 99, 4597-4610.	3.1	3,923
3	Relativistic total energy using regular approximations. Journal of Chemical Physics, 1994, 101, 9783-9792.	3.1	2,924
4	Towards an order-. Theoretical Chemistry Accounts, 1998, 99, 391.	1.5	2,454
5	Optimized Slater-type basis sets for the elements 1-118. Journal of Computational Chemistry, 2003, 24, 1142-1156.	3.4	2,423
6	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.	3.1	1,513
7	Exchange-correlation potential with correct asymptotic behavior. Physical Review A, 1994, 49, 2421-2431.	2.6	1,359
8	Towards an order- N DFT method. Theoretical Chemistry Accounts, 1998, 99, 391-403.	1.5	1,298
9	Relativistic regular two-component Hamiltonians. International Journal of Quantum Chemistry, 1996, 57, 281-293.	2.1	1,062
10	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.	3.4	999
11	Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry. Reviews in Computational Chemistry, 2007, , 1-86.	0.0	941
12	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.	3.1	705
13	A Quantum Chemical View of Density Functional Theory. Journal of Physical Chemistry A, 1997, 101, 5383-5403.	2.6	585
14	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.	14.6	523
15	Interpretation of the Kohnâ€“Sham orbital energies as approximate vertical ionization potentials. Journal of Chemical Physics, 2002, 116, 1760-1772.	3.1	484
16	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.	3.1	468
17	Precise density-functional method for periodic structures. Physical Review B, 1991, 44, 7888-7903.	3.3	464
18	Hydrogen Bonding in DNA Base Pairs:â€‰ Reconciliation of Theory and Experiment. Journal of the American Chemical Society, 2000, 122, 4117-4128.	14.6	424

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19	Binding energy and electronic structure of small copper particles. Physical Review B, 1983, 27, 2132-2144.	3.3	395
20	Chiroptical properties from time-dependent density functional theory. I. Circular dichroism spectra of organic molecules. Journal of Chemical Physics, 2002, 116, 6930-6940.	3.1	390
21	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.	2.9	367
22	Calculation of bond energies in compounds of heavy elements by a quasi-relativistic approach. The Journal of Physical Chemistry, 1989, 93, 3050-3056.	3.0	358
23	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.	3.1	345
24	Electric Field Dependence of the Exchange-Correlation Potential in Molecular Chains. Physical Review Letters, 1999, 83, 694-697.	8.0	342
25	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.	3.9	342
26	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.	14.6	334
27	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.	3.1	328
28	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.	3.1	316
29	The Carbonâ^'Lithium Electron Pair Bond in (CH3Li)n(n= 1, 2, 4). Organometallics, 1996, 15, 2923-2931.	2.6	291
30	Relativistic effects on bonding. Journal of Chemical Physics, 1981, 74, 1271-1284.	3.1	259
31	An approximate exchange-correlation hole density as a functional of the natural orbitals. Molecular Physics, 2002, 100, 401-421.	1.7	253
32	Density-functional-theory response-property calculations with accurate exchange-correlation potentials. Physical Review A, 1998, 57, 2556-2571.	2.6	250
33	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.	3.1	244
34	Self-consistent approximation to the Kohn-Sham exchange potential. Physical Review A, 1995, 51, 1944-1954.	2.6	242
35	Ground State of the (H2O)2+ Radical Cation:â€‰ DFT versus Post-Hartreeâ^'Fock Methods. Journal of Physical Chemistry A, 1999, 103, 166-170.	2.6	234
36	The Case for Steric Repulsion Causing the Staggered Conformation of Ethane. Angewandte Chemie - International Edition, 2003, 42, 4183-4188.	14.7	227

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37	Even-tempered slater-type orbitals revisited: From hydrogen to krypton. Journal of Computational Chemistry, 2004, 25, 1030-1036.	3.4	220
38	Cohesive energy of 3dtransition metals: Density functional theory atomic and bulk calculations. Physical Review B, 1996, 54, 5326-5333.	3.3	210
39	The merits of the frozen-density embedding scheme to model solvatochromic shifts. Journal of Chemical Physics, 2005, 122, 094115.	3.1	209
40	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.	2.6	202
41	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.	5.6	201
42	Atomic and molecular hydrogen interacting with Pt(111). Journal of Chemical Physics, 1999, 111, 11155-11163.	3.1	198
43	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.	3.1	197
44	Calculating frequency-dependent hyperpolarizabilities using time-dependent density functional theory. Journal of Chemical Physics, 1998, 109, 10644-10656.	3.1	196
45	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.	3.0	193
46	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	2.7	193
47	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.	3.1	192
48	Time-dependent Density Functional Results for the Dynamic Hyperpolarizability ofC60. Physical Review Letters, 1997, 78, 3097-3100.	8.0	187
49	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.	3.1	187
50	Fenton-like Chemistry in Water:Â Oxidation Catalysis by Fe(III) and H2O2. Journal of Physical Chemistry A, 2003, 107, 5722-5731.	2.6	184
51	An improved density matrix functional by physically motivated repulsive corrections. Journal of Chemical Physics, 2005, 122, 204102.	3.1	179
52	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.	3.9	172
53	Time-dependent density functional calculations on the electronic absorption spectrum of free base porphin. Journal of Chemical Physics, 1999, 111, 2499-2506.	3.1	169
54	Accurate density functional calculations on frequency-dependent hyperpolarizabilities of small molecules. Journal of Chemical Physics, 1998, 109, 10657-10668.	3.1	167

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55	The Mechanism of Zinc(II)-Dithiocarbamate-Accelerated Vulcanization Uncovered; Theoretical and Experimental Evidence. Journal of the American Chemical Society, 1999, 121, 163-168.	14.6	167
56	Can the Counterpoise Correction for Basis Set Superposition Effect Be Justified?. Journal of Chemical Theory and Computation, 2014, 10, 252-267.	5.6	167
57	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.	3.3	165
58	Metal-Macrocycle Interaction in Phthalocyanines: Density Functional Calculations of Ground and Excited States. Inorganic Chemistry, 1994, 33, 584-595.	4.2	156
59	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, .	2.6	156
60	Analysis of electron interaction and atomic shell structure in terms of local potentials. Journal of Chemical Physics, 1994, 101, 8955-8963.	3.1	154
61	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.	2.6	152
62	Analysis of correlation in terms of exact local potentials: Applications to two-electron systems. Physical Review A, 1989, 40, 4190-4202.	2.6	148
63	Exact solutions of regular approximate relativistic wave equations for hydrogenâ€like atoms. Journal of Chemical Physics, 1994, 101, 1272-1281.	3.1	145
64	Ethylene epoxidation on silver(110): the role of subsurface oxygen. The Journal of Physical Chemistry, 1989, 93, 6469-6475.	3.0	143
65	Relativistic atomic orbital contractions and expansions: magnitudes and explanations. Journal of Physics B: Atomic, Molecular and Optical Physics, 1990, 23, 3225-3240.	1.6	141
66	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.	3.1	137
67	DFT Study of the Active Intermediate in the Fenton Reaction. Chemistry - A European Journal, 2001, 7, 2775-2783.	3.9	136
68	Ground and Excited States of Zinc Phthalocyanine Studied by Density Functional Methods. Journal of Physical Chemistry A, 2001, 105, 5242-5254.	2.6	133
69	Cluster studies of CO adsorption. III. CO on small Cu clusters. Journal of Chemical Physics, 1983, 78, 5663-5681.	3.1	131
70	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.	2.6	131
71	An Explicit Quantum Chemical Method for Modeling Large Solvation Shells Applied to Aminocoumarin C151. Journal of Physical Chemistry A, 2005, 109, 7805-7814.	2.6	131
72	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.	3.0	127

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73	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.	1.5	127
74	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.	2.6	127
75	Six-Dimensional Quantum Dynamics of Dissociative Chemisorption of (v=0,j=0)H2on Cu(100). Physical Review Letters, 1997, 78, 3583-3586.	8.0	126
76	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.	3.1	126
77	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.	3.1	122
78	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.	3.1	122
79	DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science. Physical Chemistry Chemical Physics, 2022, 24, 28700-28781.	2.9	122
80	Exact Exchange-Correlation Treatment of DissociatedH2in Density Functional Theory. Physical Review Letters, 2001, 87, 133004.	8.0	121
81	An analytical sixâ€dimensional potential energy surface for dissociation of molecular hydrogen on Cu(100). Journal of Chemical Physics, 1996, 104, 7344-7358.	3.1	120
82	Nucleophilic or Electrophilic Phosphinidene Complexes MLnPH; What Makes the Difference?. Journal of the American Chemical Society, 2002, 124, 2831-2838.	14.6	117
83	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.	3.1	114
84	Quadratic integration over the three-dimensional Brillouin zone. Journal of Physics Condensed Matter, 1991, 3, 6721-6742.	1.9	112
85	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.	3.1	111
86	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.	14.6	109
87	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.	2.1	108
88	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.	3.1	106
89	Effect of molecular dissociation on the exchange-correlation Kohn-Sham potential. Physical Review A, 1996, 54, 1957-1972.	2.6	106
90	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.	3.1	106

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91	Molecular Kohn-Sham exchange-correlation potential from the correlatedab initioelectron density. Physical Review A, 1995, 52, 1870-1874.	2.6	104
92	CO on Pt(111): A puzzle revisited. Journal of Chemical Physics, 2003, 119, 4522-4528.	3.1	103
93	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.	2.2	103
94	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.	14.6	102
95	Dissociation Energies, Vibrational Frequencies, and13C NMR Chemical Shifts of the 18-Electron Species [M(CO)6]n(M = Hfâ^'Ir, Mo, Tc, Ru, Cr, Mn, Fe). A Density Functional Study. Inorganic Chemistry, 1997, 36, 5031-5036.	4.2	100
96	The analog of Koopmansâ€™ theorem in spin-density functional theory. Journal of Chemical Physics, 2002, 117, 9154-9159.	3.1	100
97	A density matrix functional with occupation number driven treatment of dynamical and nondynamical correlation. Journal of Chemical Physics, 2008, 129, 164105.	3.1	99
98	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.	14.6	93
99	The origin of relativistic effects of atomic orbitals. Journal of Physics B: Atomic, Molecular and Optical Physics, 1989, 22, 1515-1529.	1.6	91
100	Solvation Effects on the SN2 Reaction between CH3Cl and Cl-in Water. Journal of Physical Chemistry A, 2001, 105, 3300-3310.	2.6	91
101	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.	3.1	91
102	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.	3.1	90
103	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.	4.2	90
104	MSi2/Si(111) (M=Co,Ni) interface chemical bond. Physical Review Letters, 1988, 60, 1743-1746.	8.0	89
105	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.	14.6	88
106	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.	4.2	87
107	Time-dependent density-matrix-functional theory. Physical Review A, 2007, 75, .	2.6	87
108	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.	1.5	87

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109	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.	3.9	86
110	Perspective on "Self-consistent equations including exchange and correlation effects". Theoretical Chemistry Accounts, 2000, 103, 265-269.	1.5	86
111	Robust normal modes in vibrational circular dichroism spectra. Physical Chemistry Chemical Physics, 2009, 11, 6107.	2.9	85
112	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.	2.6	84
113	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.	2.9	84
114	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.	3.1	84
115	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.	3.1	81
116	O2 Evolution in the Fenton Reaction. Chemistry - A European Journal, 2003, 9, 3436-3444.	3.9	81
117	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.	3.1	81
118	Synergism of Porphyrin-Core Saddling and Twisting ofmeso-Aryl Substituents. Journal of Physical Chemistry A, 2006, 110, 5180-5190.	2.6	81
119	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.	3.1	80
120	Calculation of harmonic frequencies and harmonic force fields by the hartree-fock-slater method. International Journal of Quantum Chemistry, 1988, 34, 173-181.	2.1	79
121	Dissociation of H2on Cu(100): Dynamics on a new twoâ€•dimensional potential energy surface. Journal of Chemical Physics, 1995, 102, 3873-3883.	3.1	79
122	A Theoretical study of the interaction of ethylene with transition metal complexes. Theoretical Chemistry Accounts, 1972, 27, 339-354.	1.5	77
123	Six-dimensional quantum dynamics of dissociative chemisorption of H2 on Cu(100). Journal of Chemical Physics, 1997, 107, 3309-3323.	3.1	77
124	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.	3.1	76
125	A theoretical study of the linear versus bent geometry for several MX2 molecules: MgF2, CaH2, CaF2, CeO2 and YbCl2. Polyhedron, 1990, 9, 1919-1934.	2.3	75
126	Effects of Complex Formation on Vibrational Circular Dichroism Spectra. Journal of Physical Chemistry A, 2008, 112, 6978-6991.	2.6	75

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127	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.	2.6	74
128	Excitation Energies of Metal Complexes with Time-dependent Density Functional Theory. Structure and Bonding, 2004, , 49-116.	0.0	74
129	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.	2.3	73
130	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.	2.6	73
131	Electronic spectrum of UO22+ and [UO2Cl4]2â^' calculated with time-dependent density functional theory. Journal of Chemical Physics, 2007, 126, 194311.	3.1	73
132	Charge Transfer, Double and Bond-Breaking Excitations with Time-Dependent Density Matrix Functional Theory. Physical Review Letters, 2008, 101, 033004.	8.0	73
133	Kohn-Sham potentials corresponding to Slater and Gaussian basis set densities. Theoretical Chemistry Accounts, 1997, 98, 16-24.	1.5	72
134	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.	4.2	71
135	Energetics of intermediates and reaction steps involved in the hydroformylation reaction catalyzed by HCo(CO)4. A theoretical study based on density functional theory. Journal of the American Chemical Society, 1989, 111, 2018-2025.	14.6	69
136	Towards excitation energies and (hyper)polarizability calculations of large molecules. Application of parallelization and linear scaling techniques to time-dependent density functional response theory. Journal of Computational Chemistry, 2000, 21, 1511-1523.	3.4	68
137	Energy expressions in density-functional theory using line integrals. Physical Review A, 1995, 51, 170-178.	2.6	67
138	Bonding Properties of a Novel Inorganometallic Complex, Ru(SnPh3)2(CO)2(iPr-DAB) (iPr-DAB) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 31 Spectroscopy, (Spectro-) Electrochemistry, and Density Functional Calculations. Inorganic Chemistry, 1996, 35, 5468-5477.	4.2	67
139	Relativistic calculations to assess the ability of the generalized gradient approximation to reproduce trends in cohesive properties of solids. Physical Review B, 2000, 61, 1773-1778.	3.3	67
140	Reaction Path Sampling of the Reaction between Iron(II) and Hydrogen Peroxide in Aqueous Solution. Journal of Physical Chemistry A, 2002, 106, 7902-7910.	2.6	67
141	Vibronic Structure of the Permanganate Absorption Spectrum from Time-Dependent Density Functional Calculations. Journal of Physical Chemistry A, 2005, 109, 1168-1179.	2.6	66
142	Adsorption and diffusion on a stepped surface: Atomic hydrogen on Pt(211). Journal of Chemical Physics, 2004, 120, 11852-11863.	3.1	65
143	Modeling solvent effects on electron-spin-resonance hyperfine couplings by frozen-density embedding. Journal of Chemical Physics, 2005, 123, 114101.	3.1	65
144	X-ray Structure of fac-IMn(CO)3(bpy) and Electronic Structures and Transitions of the Complexes fac-XMn(CO)3(bpy) (X = Cl, I) and mer-ClMn(CO)3(bpy). Inorganic Chemistry, 1995, 34, 1588-1594.	4.2	64

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145	Density Functional Study of the Photodissociation of Mn2(CO)10. Inorganic Chemistry, 1996, 35, 2886-2897.	4.2	64
146	The EDTA Complex of Oxidoiron(IV) as Realisation of an Optimal Ligand Environment for High Activity of FeO²⁺. European Journal of Inorganic Chemistry, 2008, 2008, 1672-1681.	2.2	63
147	A VCD robust mode analysis of induced chirality: The case of pulegone in chloroform. Chirality, 2009, 21, E287-97.	2.7	63
148	Model systems for initial stages in oxidative-addition reactions. Theoretical investigation of .eta.1 and .eta.2 coordination of difluorine and dihydrogen to tetrachloroplatinate(2-) and chromium pentacarbonyl. Inorganic Chemistry, 1990, 29, 350-354.	4.2	62
149	Mechanisms of H2 dissociative adsorption on the Pt(211) stepped surface. Journal of Chemical Physics, 2005, 122, 194708.	3.1	62
150	Oxidative properties of FeO2+: electronic structure and solvation effects. Physical Chemistry Chemical Physics, 2007, 9, 156-166.	2.9	62
151	Analytic quadratic integration over the two-dimensional Brillouin zone. Journal of Physics C: Solid State Physics, 1988, 21, 4263-4283.	1.5	61
152	Origin and relevance of the staggering in one-dimensional molecular metals. A density functional study of metallophthalocyanine model dimers. Inorganic Chemistry, 1992, 31, 4717-4726.	4.2	61
153	Step structure in the atomic Kohn-Sham potential. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1995, 33, 229-238.	1.0	61
154	Four component regular relativistic Hamiltonians and the perturbational treatment of Diracâ€™s equation. Journal of Chemical Physics, 1995, 102, 1758-1766.	3.1	61
155	Might BF and BNR2 be alternatives to CO? A theoretical quest for new ligands in organometallic chemistry. New Journal of Chemistry, 1998, 22, 1-3.	2.7	61
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