Evert Jan Baerends

List of Publications by Year
in descending order

350 papers	55,869 citations	2046 97 h-index	981 230 g-index
373 all docs	373 docs citations	373 times ranked	20829 citing authors

#	Article	IF	Citations
1	Dispersion Energies with the i-DMFT Method. Journal of Chemical Theory and Computation, 2024, 20, 5466-5474.	5.4	0
2	Self-Consistent-Field Method for Correlated Many-Electron Systems with an Entropic Cumulant Energy. Physical Review Letters, 2022, 128, 013001.	7.8	27
3	Chemical potential, derivative discontinuity, fractional electrons, jump of the Kohnâ€“Sham potential, atoms as thermodynamic open systems, and other (mis)conceptions of the density functional theory of electrons in molecules. Physical Chemistry Chemical Physics, 2022, 24, 12745-12766.	2.8	13
4	Secondary Kinetic Peak in the Kohnâ€“Sham Potential and Its Connection to the Response Step. Journal of Chemical Theory and Computation, 2022, 18, 4762-4773.	5.4	3
5	DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science. Physical Chemistry Chemical Physics, 2022, 24, 28700-28781.	2.8	122
6	On derivatives of the energy with respect to total electron number and orbital occupation numbers. A critique of Janak's theorem. Molecular Physics, 2020, 118, .	1.7	19
7	The Electron Affinity as the Highest Occupied Anion Orbital Energy with a Sufficiently Accurate Approximation of the Exact Kohnâ€“Sham Potential. Journal of Chemical Theory and Computation, 2020, 16, 443-452.	5.4	25
8	Origin of the Enhanced Binding Capability toward Axial Nitrogen Bases of Ni(II) Porphyrins Bearing Electron-Withdrawing Substituents: An Electronic Structure and Bond Energy Analysis. Inorganic Chemistry, 2020, 59, 11528-11541.	4.1	4
9	A non-JKL density matrix functional for intergeminal correlation between closed-shell geminals from analysis of natural orbital configuration interaction expansions. Journal of Chemical Physics, 2018, 148, 104102.	2.9	18
10	Asymptotic nodal planes in the electron density and the potential in the effective equation for the square root of the density. European Physical Journal B, 2018, 91, 1.	1.5	14
11	Density functional approximations for orbital energies and total energies of molecules and solids. Journal of Chemical Physics, 2018, 149, 054105.	2.9	35
12	Natural excitation orbitals from linear response theories: Time-dependent density functional theory, time-dependent Hartree-Fock, and time-dependent natural orbital functional theory. Journal of Chemical Physics, 2017, 146, 044119.	2.9	10
13	Catalytic Oxidation of Water with High-Spin Iron(IV)â€“Oxo Species: Role of the Water Solvent. ACS Catalysis, 2017, 7, 4018-4025.	11.3	40
14	From the Kohnâ€“Sham band gap to the fundamental gap in solids. An integer electron approach. Physical Chemistry Chemical Physics, 2017, 19, 15639-15656.	2.8	44
15	Comment on â€œKohn-Sham exchange-correlation potentials from second-order reduced density matricesâ€•[J. Chem. Phys. 143, 244116 (2015)]. Journal of Chemical Physics, 2016, 145, 037101.	2.9	11
16	On the errors of local density (LDA) and generalized gradient (GGA) approximations to the Kohn-Sham potential and orbital energies. Journal of Chemical Physics, 2016, 144, 204114.	2.9	51
17	Time-dependent Dyson orbital theory. Physical Chemistry Chemical Physics, 2016, 18, 20945-20954.	2.8	3
18	Asymptotic behaviour of the electron density and the Kohnâ€“Sham potential in case of a Kohnâ€“Sham HOMO nodal plane. Molecular Physics, 2016, 114, 1086-1097.	1.7	24

#	Article	IF	Citations
19	Charge Effects on the Reactivity of Oxoiron(IV) Porphyrin Species: A DFT Analysis of Methane Hydroxylation by Polycationic Compound I and Compound II Mimics. ACS Catalysis, 2016, 6, 568-579.	11.3	28
20	Ligand Field Effects and the High Spinâ€“High Reactivity Correlation in the H Abstraction by Non-Heme Iron(IV)â€“Oxo Complexes: A DFT Frontier Orbital Perspective. ACS Catalysis, 2015, 5, 1475-1488.	11.3	45
21	Light-induced water splitting by titanium-tetrahydroxide: a computational study. Physical Chemistry Chemical Physics, 2015, 17, 20308-20321.	2.8	16
22	Real-space representation of electron correlation in Ï€-conjugated systems. Journal of Chemical Physics, 2015, 142, 204311.	2.9	3
23	The density matrix functional approach to electron correlation: Dynamic and nondynamic correlation along the full dissociation coordinate. Journal of Chemical Physics, 2014, 140, 214105.	2.9	31
24	Response calculations based on an independent particle system with the exact one-particle density matrix: Polarizabilities. Journal of Chemical Physics, 2014, 140, 18A517.	2.9	7
25	Solvent induced enhancement of enantiomeric excess: a case study of the Henry reaction with cinchona thiourea as the catalyst. Physical Chemistry Chemical Physics, 2014, 16, 7315.	2.8	10
26	Excitation energies with linear response density matrix functional theory along the dissociation coordinate of an electron-pair bond in N-electron systems. Journal of Chemical Physics, 2014, 140, 024101.	2.9	16
27	Can the Counterpoise Correction for Basis Set Superposition Effect Be Justified?. Journal of Chemical Theory and Computation, 2014, 10, 252-267.	5.4	167
28	The Importance of Large-Amplitude Motions for the Interpretation of Mid-Infrared Vibrational Absorption and Circular Dichroism Spectra: 6,6â€²-Dibromo-[1,1â€²-binaphthalene]-2,2â€²-diol in Dimethyl Sulfoxide. Journal of Physical Chemistry A, 2014, 118, 4766-4777.	2.5	24
29	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.	5.4	201
30	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	367
31	Assessment of density functional methods for reaction energetics: Iridiumâ€catalyzed water oxidation as case study. Journal of Computational Chemistry, 2013, 34, 870-878.	3.4	29
32	A natural orbital analysis of the long range behavior of chemical bonding and van der Waals interaction in singlet H2: The issue of zero natural orbital occupation numbers. Journal of Chemical Physics, 2013, 138, 164105.	2.9	17
33	A Frontier Orbital Study with ab Initio Molecular Dynamics of the Effects of Solvation on Chemical Reactivity: Solvent-Induced Orbital Control in FeO-Activated Hydroxylation Reactions. Journal of the American Chemical Society, 2013, 135, 8857-8867.	14.1	42
34	Oscillator strengths of electronic excitations with response theory using phase including natural orbital functionals. Journal of Chemical Physics, 2013, 138, 094114.	2.9	19
35	Response calculations based on an independent particle system with the exact one-particle density matrix: Excitation energies. Journal of Chemical Physics, 2012, 136, 094104.	2.9	35
36	Hydroxylation Catalysis by Mononuclear and Dinuclear Iron Oxo Catalysts: a Methane Monooxygenase Model System versus the Fenton Reagent Fe^{IV}O(H₂O)₅²⁺. Inorganic Chemistry, 2012, 51, 63-75.	4.1	24

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37	Understanding Solvent Effects in Vibrational Circular Dichroism Spectra: [1,1â€²-Binaphthalene]-2,2â€²-diol in Dichloromethane, Acetonitrile, and Dimethyl Sulfoxide Solvents. Journal of Physical Chemistry A, 2012, 116, 8366-8373.	2.5	59
38	On the formulation of a density matrix functional for Van der Waals interaction of like- and opposite-spin electrons in the helium dimer. Journal of Chemical Physics, 2012, 137, 204117.	2.9	8
39	Titanium as a Potential Addition for High-Capacity Hydrogen Storage Medium. Journal of Nanotechnology, 2012, 2012, 1-9.	3.5	7
40	On the Equivalence of Conformational and Enantiomeric Changes of Atomic Configuration for Vibrational Circular Dichroism Signs. Journal of Physical Chemistry A, 2012, 116, 3454-3464.	2.5	12
41	An abiotic analogue of the diiron(iv)oxo â€œdiamond coreâ€•of soluble methane monooxygenase generated by direct activation of O2 in aqueous Fe(ii)/EDTA solutions: thermodynamics and electronic structure. Physical Chemistry Chemical Physics, 2011, 13, 15272.	2.8	15
42	On the origin dependence of the angle made by the electric and magnetic vibrational transition dipole moment vectors. Physical Chemistry Chemical Physics, 2011, 13, 16126.	2.8	23
43	Electron pair density in the lowest1Î£u+ and1Î£g+ states of H2. Journal of Chemical Physics, 2011, 135, 074111.	2.9	6
44	Cu(bipy)²⁺/TEMPO-Catalyzed Oxidation of Alcohols: Radical or Nonradical Mechanism?. Inorganic Chemistry, 2011, 50, 11896-11904.	4.1	43
45	Diffractive and reactive scattering of H2 from Ru(0001): experimental and theoretical study. Physical Chemistry Chemical Physics, 2011, 13, 8583.	2.8	32
46	Counterpoise correction is not useful for short and Van der Waals distances but may be useful at long range. Journal of Computational Chemistry, 2011, 32, 2896-2901.	3.4	52
47	Signatures of counter-ion association and hydrogen bonding in vibrational circular dichroism spectra. Physical Chemistry Chemical Physics, 2011, 13, 8811.	2.8	26
48	Complexation, Solvation, and Chirality Transfer in Vibrational Circular Dichroism. , 2011, , 747-781.		1
49	The adiabatic approximation in time-dependent density matrix functional theory: Response properties from dynamics of phase-including natural orbitals. Journal of Chemical Physics, 2010, 133, 174119.	2.9	29
50	Counterintuitive Coulomb hole around the bond midplane. Journal of Chemical Physics, 2010, 132, 204102.	2.9	8
51	Aufbau derived from a unified treatment of occupation numbers in Hartreeâ€“Fock, Kohnâ€“Sham, and natural orbital theories with the Karushâ€“Kuhnâ€“Tucker conditions for the inequality constraints niâ‰¤1 and niâ‰¥. Journal of Chemical Physics, 2010, 132, 194108.	2.9	42
52	Response Calculations with an Independent Particle System with an Exact One-Particle Density Matrix. Physical Review Letters, 2010, 105, 013002.	7.8	42
53	A new analytical potential energy surface for the adsorption system CO/Cu(100). Journal of Chemical Physics, 2010, 132, 074108.	2.9	29
54	Is [FeO]²⁺ the Active Center Also in Iron Containing Zeolites? A Density Functional Theory Study of Methane Hydroxylation Catalysis by Fe-ZSM-5 Zeolite. Inorganic Chemistry, 2010, 49, 3866-3880.	4.1	54

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55	Generation of Ferryl Species through Dioxygen Activation in Iron/EDTA Systems: A Computational Study. Inorganic Chemistry, 2009, 48, 527-540.	4.1	32
56	A VCD robust mode analysis of induced chirality: The case of pulegone in chloroform. Chirality, 2009, 21, E287-97.	2.7	63
57	Homolytic versus Heterolytic Dissociation of Alkalimetal Halides: The Effect of Microsolvation. ChemPhysChem, 2009, 10, 2955-2965.	2.3	14
58	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.	4.1	71
59	O₂ Activation in a Dinuclear Fe(II)/EDTA Complex: Spin Surface Crossing As a Route to Highly Reactive Fe(IV)oxo Species. Journal of Physical Chemistry A, 2009, 113, 11926-11937.	2.5	34
60	Excitation energies with time-dependent density matrix functional theory: Singlet two-electron systems. Journal of Chemical Physics, 2009, 130, 114104.	2.9	55
61	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.	4.1	90
62	The analog of Koopmansâ€™ theorem for virtual Kohnâ€“Sham orbital energies. Canadian Journal of Chemistry, 2009, 87, 1383-1391.	1.1	30
63	Double excitation effect in non-adiabatic time-dependent density functional theory with an analytic construction of the exchangeâ€“correlation kernel in the common energy denominator approximation. Physical Chemistry Chemical Physics, 2009, 11, 4640.	2.8	45
64	Robust normal modes in vibrational circular dichroism spectra. Physical Chemistry Chemical Physics, 2009, 11, 6107.	2.8	85
65	Suitability of III-V<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>[</mml:mo><mml:mrow><mml:mi>X</mml:mi><mml:msub><mml:mtext>H</mml:mtext> for hydrogen storage: A density functional study. Physical Review B, 2009, 79, .	3.2	6
66	Enhancement of IR and VCD intensities due to charge transfer. Physical Chemistry Chemical Physics, 2009, 11, 1526.	2.8	56
67	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
68	Density functional theory calculation of 2p spectra of SiH₄, PH₃, H₂S, HCl, and Ar. International Journal of Quantum Chemistry, 2008, 108, 1358-1368.	2.1	5
69	Influence of the Copper Coordination Geometry on the DNA Cleavage Activity of Clip-Phen Complexes Studied by DFT. European Journal of Inorganic Chemistry, 2008, 2008, 612-619.	2.2	24
70	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
71	Oxidation of Methanol by FeO²⁺ in Water:â€‰ DFT Calculations in the Gas Phase and Ab Initio MD Simulations in Water Solution. Journal of Physical Chemistry A, 2008, 112, 1000-1012.	2.5	45
72	Effects of Complex Formation on Vibrational Circular Dichroism Spectra. Journal of Physical Chemistry A, 2008, 112, 6978-6991.	2.5	75

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73	A density matrix functional with occupation number driven treatment of dynamical and nondynamical correlation. Journal of Chemical Physics, 2008, 129, 164105.	2.9	99
74	Six-dimensional quantum dynamics of H2 dissociative adsorption on the Pt(211) stepped surface. Journal of Chemical Physics, 2008, 128, 194715.	2.9	29
75	Charge Transfer, Double and Bond-Breaking Excitations with Time-Dependent Density Matrix Functional Theory. Physical Review Letters, 2008, 101, 033004.	7.8	73
76	Electronic spectrum of UO22+ and [UO2Cl4]2â^' calculated with time-dependent density functional theory. Journal of Chemical Physics, 2007, 126, 194311.	2.9	73
77	Time-dependent density-matrix-functional theory. Physical Review A, 2007, 75, .	2.5	87
78	Oxidative properties of FeO2+: electronic structure and solvation effects. Physical Chemistry Chemical Physics, 2007, 9, 156-166.	2.8	62
79	Adiabatic approximation of time-dependent density matrix functional response theory. Journal of Chemical Physics, 2007, 127, 214101.	2.9	41
80	Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry. Reviews in Computational Chemistry, 2007, , 1-86.	0.0	941
81	A Square-Planar Nickel(II) Monoradical Complex with a Bis(salicylidene)diamine Ligand. European Journal of Inorganic Chemistry, 2007, 2007, 637-642.	2.2	46
82	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
83	First Hyperpolarizability of a Sesquifulvalene Transition Metal Complex by Time-Dependent Density-Functional Theory. Journal of Physical Chemistry A, 2006, 110, 1014-1021.	2.5	26
84	Six-dimensional potential energy surface for H2at Ru(0001). Physical Chemistry Chemical Physics, 2006, 8, 688-696.	2.8	40
85	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	2.6	193
86	Synergism of Porphyrin-Core Saddling and Twisting ofmeso-Aryl Substituents. Journal of Physical Chemistry A, 2006, 110, 5180-5190.	2.5	81
87	Exploring the Ability of Frozen-Density Embedding to Model Induced Circular Dichroism. Journal of Physical Chemistry A, 2006, 110, 8786-8796.	2.5	52
88	Role of the Fermi Surface in Adsorbateâ^'Metal Interactions:Â An Energy Decomposition Analysis. Journal of Physical Chemistry B, 2006, 110, 12470-12479.	2.6	14
89	Long-Range Solvent Effects on the Orbital Interaction Mechanism of Water Acidity Enhancement in Metal Ion Solutions:Â A Comparative Study of the Electronic Structure of Aqueous Mg and Zn Dications. Journal of Physical Chemistry B, 2006, 110, 11444-11453.	2.6	43
90	Orbital interactions and charge redistribution in weak hydrogen bonds: Watson-Crick GC mimic involving Cï£¿H proton donor and F proton acceptor groups. International Journal of Quantum Chemistry, 2006, 106, 2428-2443.	2.1	8

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91	Correct dissociation limit for the exchange-correlation energy and potential. International Journal of Quantum Chemistry, 2006, 106, 3167-3177.	2.1	15
92	Calculation of pressure in case of periodic boundary conditions. Chemical Physics Letters, 2006, 421, 138-141.	2.6	56
93	Variational collapse of the optimized effective potential method with an orbital-dependent exchange-correlation functional based on second order perturbation theory. Chemical Physics Letters, 2006, 432, 336-342.	2.6	17
94	Precision of total energy and orbital energies with the expansion method for the optimized effective Kohnâ€“Sham potential. Computational and Theoretical Chemistry, 2006, 762, 193-199.	1.5	22
95	A simple natural orbital mechanism of â€œpureâ€•van der Waals interaction in the lowest excited triplet state of the hydrogen molecule. Journal of Chemical Physics, 2006, 124, 054115.	2.9	22
96	Coupled-perturbed density-matrix functional theory equations. Application to static polarizabilities. Journal of Chemical Physics, 2006, 124, 014102.	2.9	19
97	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.	2.9	126
98	Away from generalized gradient approximation: Orbital-dependent exchange-correlation functionals. Journal of Chemical Physics, 2005, 123, 062202.	2.9	58
99	An improved density matrix functional by physically motivated repulsive corrections. Journal of Chemical Physics, 2005, 122, 204102.	2.9	179
100	Rotational effects in the dissociative adsorption of H2 on the Pt(211) stepped surface. Journal of Chemical Physics, 2005, 123, 164702.	2.9	22
101	Importance of vibronic effects on the circular dichroism spectrum of dimethyloxirane. Journal of Chemical Physics, 2005, 122, 234305.	2.9	54
102	Mechanisms of H2 dissociative adsorption on the Pt(211) stepped surface. Journal of Chemical Physics, 2005, 122, 194708.	2.9	62
103	The merits of the frozen-density embedding scheme to model solvatochromic shifts. Journal of Chemical Physics, 2005, 122, 094115.	2.9	209
104	The uranyl ion revisited: the electric field gradient at U as a probe of environmental effects. Molecular Physics, 2005, 103, 775-787.	1.7	13
105	Combined Theoretical and Experimental Deep-UV Resonance Raman Studies of Substituted Pyrenes. Journal of Physical Chemistry A, 2005, 109, 2100-2106.	2.5	59
106	Hydroxyl Radical and Hydroxide Ion in Liquid Water:â€‰ A Comparative Electron Density Functional Theory Study. Journal of Physical Chemistry B, 2005, 109, 23605-23610.	2.6	50
107	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	131
108	Vibronic Structure of the Permanganate Absorption Spectrum from Time-Dependent Density Functional Calculations. Journal of Physical Chemistry A, 2005, 109, 1168-1179.	2.5	66

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109	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.	2.9	244
110	Modeling solvent effects on electron-spin-resonance hyperfine couplings by frozen-density embedding. Journal of Chemical Physics, 2005, 123, 114101.	2.9	65
111	Structural, Optical, and Photophysical Properties of Nickel(II) Alkylthioporphyrins:Â Insights from Experimental and DFT/TDDFT Studies. Inorganic Chemistry, 2005, 44, 6609-6622.	4.1	49
112	Photophysics of Octabutoxy Phthalocyaninato-Ni(II) in Toluene:Â Ultrafast Experiments and DFT/TDDFT Studies. Journal of Physical Chemistry A, 2005, 109, 2078-2089.	2.5	55
113	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.	2.9	81
114	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.	2.9	328
115	Reactive scattering of H[sub 2] from Cu(100): Six-dimensional quantum dynamics results for reaction and scattering obtained with a new, accurately fitted potential-energy surface. Journal of Chemical Physics, 2004, 121, 11379.	2.9	26
116	Adsorption and diffusion on a stepped surface: Atomic hydrogen on Pt(211). Journal of Chemical Physics, 2004, 120, 11852-11863.	2.9	65
117	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.	2.9	84
118	Improving numerical integration through basis set expansion. Theoretical Chemistry Accounts, 2004, 112, 410-418.	1.4	4
119	Hydrogen Bonding in Mimics of Watsonâ€“Crick Base Pairs Involving Cï£¿H Proton Donor and F Proton Acceptor Groups: A Theoretical Study. ChemPhysChem, 2004, 5, 481-487.	2.3	41
120	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
121	Even-tempered slater-type orbitals revisited: From hydrogen to krypton. Journal of Computational Chemistry, 2004, 25, 1030-1036.	3.4	220
122	Ab initio molecular dynamics simulation of the OH radical in liquid water. Chemical Physics Letters, 2004, 398, 212-216.	2.6	50
123	The calculation of ESR parameters by density functional theory: the g- and A-tensors of Co(acacen). Chemical Physics Letters, 2004, 399, 433-439.	2.6	47
124	Improved Description of Chemical Barriers with Generalized Gradient Approximations (GGAs) and Meta-GGAs. Journal of Physical Chemistry A, 2004, 108, 4459-4469.	2.5	48
125	Exchange kernel of density functional response theory from the common energy denominator approximation (CEDA) for the Kohnâ€“Sham Green's function. Research on Chemical Intermediates, 2004, 30, 87-98.	2.7	4
126	Excitation Energies of Metal Complexes with Time-dependent Density Functional Theory. Structure and Bonding, 2004, , 49-116.	0.0	74

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127	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.	14.1	102
128	The rotation barrier in ethane. Nachrichten Aus Der Chemie, 2004, 52, 581-581.	0.0	4
129	CO on Pt(111): A puzzle revisited. Journal of Chemical Physics, 2003, 119, 4522-4528.	2.9	103
130	Optimized Slater-type basis sets for the elements 1-118. Journal of Computational Chemistry, 2003, 24, 1142-1156.	3.4	2,423
131	STO and GTO field-induced polarization functions for H to Kr. Journal of Computational Chemistry, 2003, 24, 1582-1591.	3.4	21
132	O2 Evolution in the Fenton Reaction. Chemistry - A European Journal, 2003, 9, 3436-3444.	3.8	81
133	The Case for Steric Repulsion Causing the Staggered Conformation of Ethane. Angewandte Chemie - International Edition, 2003, 42, 4183-4188.	14.2	227
134	Fenton-like Chemistry in Water:Â Oxidation Catalysis by Fe(III) and H2O2. Journal of Physical Chemistry A, 2003, 107, 5722-5731.	2.5	184
135	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
136	Nuclear magnetic resonance chemical shifts with the statistical average of orbital-dependent model potentials in Kohnâ€“Sham density functional theory. Journal of Chemical Physics, 2003, 118, 8584-8593.	2.9	48
137	Diffusion and vibration of CO molecules adsorbed on a Cu(100) surface: A periodic density functional theory study. Journal of Chemical Physics, 2003, 119, 509-514.	2.9	30
138	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.	2.9	122
139	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.	2.9	111
140	Dissociative and diffractive scattering of H2 from Pt(111): A four-dimensional quantum dynamics study. Journal of Chemical Physics, 2002, 116, 9435-9448.	2.9	29
141	Signatures of site-specific reaction of H2 on Cu(100). Journal of Chemical Physics, 2002, 117, 6673-6687.	2.9	35
142	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.	2.9	114
143	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.	2.9	91
144	Response Properties of Furan Homologues by Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2002, 106, 10380-10390.	2.5	10

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145	Orbital Interactions in Hydrogen Bonds Important for Cohesion in Molecular Crystals and Mismatched Pairs of DNA Bases. Crystal Growth and Design, 2002, 2, 239-245.	3.1	50
146	Electronic Structure, Chemical Bond, and Optical Spectra of Metal Bis(porphyrin) Complexes:Â A DFT/TDDFT Study of the Bis(porphyrin)M(IV) (M = Zr, Ce, Th) Series. Journal of the American Chemical Society, 2002, 124, 12319-12334.	14.1	54
147	The Short Nâ^'F Bond in N2F+and How Pauli Repulsion Influences Bond Lengths. Theoretical Study of N2X+, NF3X+, and NH3X+(X = F, H). Journal of the American Chemical Society, 2002, 124, 1500-1505.	14.1	54
148	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.	2.9	187
149	Chiroptical properties from time-dependent density functional theory. I. Circular dichroism spectra of organic molecules. Journal of Chemical Physics, 2002, 116, 6930-6940.	2.9	390
150	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
151	Reaction Path Sampling of the Reaction between Iron(II) and Hydrogen Peroxide in Aqueous Solution. Journal of Physical Chemistry A, 2002, 106, 7902-7910.	2.5	67
152	The analog of Koopmansâ€™ theorem in spin-density functional theory. Journal of Chemical Physics, 2002, 117, 9154-9159.	2.9	100
153	An approximate exchange-correlation hole density as a functional of the natural orbitals. Molecular Physics, 2002, 100, 401-421.	1.7	253
154	Interpretation of the Kohnâ€“Sham orbital energies as approximate vertical ionization potentials. Journal of Chemical Physics, 2002, 116, 1760-1772.	2.9	484
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