Evert Jan Baerends

List of Publications by Year in Descending Order

425 papers	60,156 citations	103 h-index	238 g-index
445 ext. papers	63,549 ext. citations	4.3 avg, IF	7.65 L-index

#	Paper	IF	Citations
425	Self-Consistent-Field Method for Correlated Many-Electron Systems with an Entropic Cumulant Energy.. *Physical Review Letters*, **2022**, 128, 013001	7.4	6
424	The Electron Affinity as the Highest Occupied Anion Orbital Energy with a Sufficiently Accurate Approximation of the Exact Kohn-Sham Potential. *Journal of Chemical Theory and Computation*, **2020**, 16, 443-452	6.4	9
423	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	5.1	3
422	On derivatives of the energy with respect to total electron number and orbital occupation numbers. A critique of Janak's theorem ** This paper honours the memory of Dieter Cremer and his penetrating analysis of fundamentals of DFT.View all notes. *Molecular Physics*, **2020**, 118, e1612955	1.7	7
421	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	3.9	14
420	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	1.2	7
419	Density functional approximations for orbital energies and total energies of molecules and solids. *Journal of Chemical Physics*, **2018**, 149, 054105	3.9	18
418	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	3.9	9
417	Catalytic Oxidation of Water with High-Spin Iron(IV)□Oxo Species: Role of the Water Solvent. *ACS Catalysis*, **2017**, 7, 4018-4025	13.1	31
416	From the Kohn-Sham band gap to the fundamental gap in solids. An integer electron approach. *Physical Chemistry Chemical Physics*, **2017**, 19, 15639-15656	3.6	37
415	Time-dependent Dyson orbital theory. *Physical Chemistry Chemical Physics*, **2016**, 18, 20945-54	3.6	3
414	Asymptotic behaviour of the electron density and the Kohn□Sham potential in case of a Kohn□Sham HOMO nodal plane. *Molecular Physics*, **2016**, 114, 1086-1097	1.7	17
413	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	13.1	20
412	Comment on "Kohn-Sham exchange-correlation potentials from second-order reduced density matrices" [J. Chem. Phys. 143, 244116 (2015)]. *Journal of Chemical Physics*, **2016**, 145, 037101	3.9	9
411	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	3.9	39
410	Light-induced water splitting by titanium-tetrahydroxide: a computational study. *Physical Chemistry Chemical Physics*, **2015**, 17, 20308-21	3.6	15
409	Real-space representation of electron correlation in □conjugated systems. *Journal of Chemical Physics*, **2015**, 142, 204311	3.9	3

408	The one-electron description of excited states: Natural excitation orbitals of density matrix theory and Kohn–Sham orbitals of density functional theory as ideal orbitals. *Chemical Physics Letters*, **2015**, 639, 315-319	2.5	8
407	Ligand Field Effects and the High Spin–High Reactivity Correlation in the H Abstraction by Non-Heme Iron(IV)–Oxo Complexes: A DFT Frontier Orbital Perspective. *ACS Catalysis*, **2015**, 5, 1475-1488	13.1	35
406	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, 7315-23	3.6	10
405	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	3.9	14
404	Can the Counterpoise Correction for Basis Set Superposition Effect Be Justified?. *Journal of Chemical Theory and Computation*, **2014**, 10, 252-67	6.4	134
403	The importance of large-amplitude motions for the interpretation of mid-infrared vibrational absorption and circular dichroism spectra: 6,6′-dibromo-[1,1′-binaphthalene]-2,2′-diol in dimethyl sulfoxide. *Journal of Physical Chemistry A*, **2014**, 118, 4766-77	2.8	18
402	Physical Meaning of Virtual Kohn-Sham Orbitals and Orbital Energies: An Ideal Basis for the Description of Molecular Excitations. *Journal of Chemical Theory and Computation*, **2014**, 10, 4432-41	6.4	155
401	The density matrix functional approach to electron correlation: dynamic and nondynamic correlation along the full dissociation coordinate. *Journal of Chemical Physics*, **2014**, 140, 214105	3.9	24
400	Response calculations based on an independent particle system with the exact one-particle density matrix: polarizabilities. *Journal of Chemical Physics*, **2014**, 140, 18A517	3.9	6
399	The Kohn-Sham gap, the fundamental gap and the optical gap: the physical meaning of occupied and virtual Kohn-Sham orbital energies. *Physical Chemistry Chemical Physics*, **2013**, 15, 16408-25	3.6	297
398	Assessment of density functional methods for reaction energetics: iridium-catalyzed water oxidation as case study. *Journal of Computational Chemistry*, **2013**, 34, 870-8	3.5	29
397	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	3.9	14
396	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, 8857-67	16.4	36
395	Oscillator strengths of electronic excitations with response theory using phase including natural orbital functionals. *Journal of Chemical Physics*, **2013**, 138, 094114	3.9	17
394	Hydroxylation catalysis by mononuclear and dinuclear iron oxo catalysts: a methane monooxygenase model system versus the Fenton reagent Fe(IV)O(H2O)5(2+). *Inorganic Chemistry*, **2012**, 51, 63-75	5.1	24
393	Understanding solvent effects in vibrational circular dichroism spectra: [1,1′-binaphthalene]-2,2′-diol in dichloromethane, acetonitrile, and dimethyl sulfoxide solvents. *Journal of Physical Chemistry A*, **2012**, 116, 8366-73	2.8	46
392	Complexation, Solvation, and Chirality Transfer in Vibrational Circular Dichroism **2012**, 747-781		1
391	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	3.9	7

390	Titanium as a Potential Addition for High-Capacity Hydrogen Storage Medium. *Journal of Nanotechnology*, **2012**, 2012, 1-9	3.5	4
389	On the equivalence of conformational and enantiomeric changes of atomic configuration for vibrational circular dichroism signs. *Journal of Physical Chemistry A*, **2012**, 116, 3454-64	2.8	12
388	Response calculations based on an independent particle system with the exact one-particle density matrix: excitation energies. *Journal of Chemical Physics*, **2012**, 136, 094104	3.9	30
387	Electron pair density in the lowest 1Π(u)(+) and 1Π(g)(+) states of H2. *Journal of Chemical Physics*, **2011**, 135, 074111	3.9	6
386	Cu(bipy)2+/TEMPO-catalyzed oxidation of alcohols: radical or nonradical mechanism?. *Inorganic Chemistry*, **2011**, 50, 11896-904	5.1	38
385	Diffractive and reactive scattering of H2 from Ru(0001): experimental and theoretical study. *Physical Chemistry Chemical Physics*, **2011**, 13, 8583-97	3.6	32
384	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, 2896-901	3.5	44
383	An abiotic analogue of the diiron(IV)oxo "diamond core" 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, 15272-82	3.6	12
382	On the origin dependence of the angle made by the electric and magnetic vibrational transition dipole moment vectors. *Physical Chemistry Chemical Physics*, **2011**, 13, 16126-9	3.6	19
381	Signatures of counter-ion association and hydrogen bonding in vibrational circular dichroism spectra. *Physical Chemistry Chemical Physics*, **2011**, 13, 8811-25	3.6	26
380	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	3.9	29
379	Counterintuitive Coulomb hole around the bond midplane. *Journal of Chemical Physics*, **2010**, 132, 204102	3.9	8
378	Aufbau derived from a unified treatment of occupation numbers in Hartree-Fock, Kohn-Sham, and natural orbital theories with the Karush-Kuhn-Tucker conditions for the inequality constraints n(i)or=0. *Journal of Chemical Physics*, **2010**, 132, 194108	3.9	34
377	Response calculations with an independent particle system with an exact one-particle density matrix. *Physical Review Letters*, **2010**, 105, 013002	7.4	38
376	A new analytical potential energy surface for the adsorption system CO/Cu(100). *Journal of Chemical Physics*, **2010**, 132, 074108	3.9	27
375	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, 3866-80	5.1	46
374	Generation of ferryl species through dioxygen activation in iron/EDTA systems: a computational study. *Inorganic Chemistry*, **2009**, 48, 527-40	5.1	28
373	A VCD robust mode analysis of induced chirality: the case of pulegone in chloroform. *Chirality*, **2009**, 21 Suppl 1, E287-97	2.1	59

372	Homolytic versus heterolytic dissociation of alkalimetal halides: the effect of microsolvation. *ChemPhysChem*, **2009**, 10, 2955-65	3.2	13
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369	Excitation energies with time-dependent density matrix functional theory: Singlet two-electron systems. *Journal of Chemical Physics*, **2009**, 130, 114104	3.9	50
368	Activation of the C-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, 11909-20	5.1	81
367	The analog of Koopmans□theorem for virtual Kohn□Sham orbital energies. *Canadian Journal of Chemistry*, **2009**, 87, 1383-1391	0.9	24
366	Double excitation effect in non-adiabatic time-dependent density functional theory with an analytic construction of the exchange-correlation kernel in the common energy denominator approximation. *Physical Chemistry Chemical Physics*, **2009**, 11, 4640-6	3.6	36
365	Robust normal modes in vibrational circular dichroism spectra. *Physical Chemistry Chemical Physics*, **2009**, 11, 6107-18	3.6	77
364	Suitability of III-V [XH4][YH4] materials for hydrogen storage: A density functional study. *Physical Review B*, **2009**, 79,	3.3	2
363	Enhancement of IR and VCD intensities due to charge transfer. *Physical Chemistry Chemical Physics*, **2009**, 11, 1526-38	3.6	50
362	Oxidation of methanol by FeO2+ in water: DFT calculations in the gas phase and ab initio MD simulations in water solution. *Journal of Physical Chemistry A*, **2008**, 112, 1000-12	2.8	38
361	Effects of complex formation on vibrational circular dichroism spectra. *Journal of Physical Chemistry A*, **2008**, 112, 6978-91	2.8	71
360	A density matrix functional with occupation number driven treatment of dynamical and nondynamical correlation. *Journal of Chemical Physics*, **2008**, 129, 164105	3.9	87
359	Six-dimensional quantum dynamics of H2 dissociative adsorption on the Pt(211) stepped surface. *Journal of Chemical Physics*, **2008**, 128, 194715	3.9	28
358	Charge transfer, double and bond-breaking excitations with time-dependent density matrix functional theory. *Physical Review Letters*, **2008**, 101, 033004	7.4	62
357	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	1.9	75
356	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	3
355	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	2.3	21

354	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	2.3	57
353	Failure of time-dependent density functional theory for excited state surfaces in case of homolytic bond dissociation. *Chemical Physics Letters*, **2008**, 461, 338-342	2.5	45
352	Watson-crick base pairs with thiocarbonyl groups: How sulfur changes the hydrogen bonds in DNA. *Open Chemistry*, **2008**, 6, 15-21	1.6	6
351	Oxidative properties of FeO2+: electronic structure and solvation effects. *Physical Chemistry Chemical Physics*, **2007**, 9, 156-66	3.6	57
350	Adiabatic approximation of time-dependent density matrix functional response theory. *Journal of Chemical Physics*, **2007**, 127, 214101	3.9	37
349	Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry. *Reviews in Computational Chemistry*, **2007**, 1-86		466
348	A Square-Planar Nickel(II) Monoradical Complex with a Bis(salicylidene)diamine Ligand. *European Journal of Inorganic Chemistry*, **2007**, 2007, 637-642	2.3	44
347	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	2.3	97
346	Electronic spectrum of UO2(2+) and [UO2Cl4]2- calculated with time-dependent density functional theory. *Journal of Chemical Physics*, **2007**, 126, 194311	3.9	61
345	Time-dependent density-matrix-functional theory. *Physical Review A*, **2007**, 75,	2.6	76
344	Polyoxometalates with internal cavities: redox activity, basicity, and cation encapsulation in [Xn+P5W30O110](15-n)- Preyssler complexes, with X = Na+, Ca2+, Y3+, La3+, Ce3+, and Th4+. *Journal of the American Chemical Society*, **2007**, 129, 12244-53	16.4	140
343	A simple natural orbital mechanism of "pure" van der Waals interaction in the lowest excited triplet state of the hydrogen molecule. *Journal of Chemical Physics*, **2006**, 124, 054115	3.9	21
342	Coupled-perturbed density-matrix functional theory equations. Application to static polarizabilities. *Journal of Chemical Physics*, **2006**, 124, 14102	3.9	17
341	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	3.9	118
340	Reactive and nonreactive scattering of H2 from a metal surface is electronically adiabatic. *Science*, **2006**, 312, 86-9	33.3	173
339	First hyperpolarizability of a sesquifulvalene transition metal complex by time-dependent density-functional theory. *Journal of Physical Chemistry A*, **2006**, 110, 1014-21	2.8	26
338	Six-dimensional potential energy surface for H2 at Ru(0001). *Physical Chemistry Chemical Physics*, **2006**, 8, 688-96	3.6	37
337	Predicting catalysis: understanding ammonia synthesis from first-principles calculations. *Journal of Physical Chemistry B*, **2006**, 110, 17719-35	3.4	168

336	Synergism of porphyrin-core saddling and twisting of meso-aryl substituents. *Journal of Physical Chemistry A*, **2006**, 110, 5180-90	2.8	73
335	Exploring the ability of frozen-density embedding to model induced circular dichroism. *Journal of Physical Chemistry A*, **2006**, 110, 8786-96	2.8	49
334	Role of the Fermi surface in adsorbate-metal interactions: an energy decomposition analysis. *Journal of Physical Chemistry B*, **2006**, 110, 12470-9	3.4	12
333	Long-range solvent effects on the orbital interaction mechanism of water acidity enhancement in metal ion solutions: a comparative study of the electronic structure of aqueous Mg and Zn dications. *Journal of Physical Chemistry B*, **2006**, 110, 11444-53	3.4	41
332	Orbital interactions and charge redistribution in weak hydrogen bonds: Watson□Crick GC mimic involving C?H proton donor and F proton acceptor groups. *International Journal of Quantum Chemistry*, **2006**, 106, 2428-2443	2.1	8
331	Correct dissociation limit for the exchange-correlation energy and potential. *International Journal of Quantum Chemistry*, **2006**, 106, 3167-3177	2.1	13
330	Calculation of pressure in case of periodic boundary conditions. *Chemical Physics Letters*, **2006**, 421, 138-141	2.1	39
329	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	2.5	17
328	Precision of total energy and orbital energies with the expansion method for the optimized effective Kohn□Sham potential. *Computational and Theoretical Chemistry*, **2006**, 762, 193-199		22
327	Combined theoretical and experimental deep-UV resonance raman studies of substituted pyrenes. *Journal of Physical Chemistry A*, **2005**, 109, 2100-6	2.8	56
326	Hydroxyl radical and hydroxide ion in liquid water: a comparative electron density functional theory study. *Journal of Physical Chemistry B*, **2005**, 109, 23605-10	3.4	43
325	An explicit quantum chemical method for modeling large solvation shells applied to aminocoumarin C151. *Journal of Physical Chemistry A*, **2005**, 109, 7805-14	2.8	120
324	Vibronic structure of the permanganate absorption spectrum from time-dependent density functional calculations. *Journal of Physical Chemistry A*, **2005**, 109, 1168-79	2.8	58
323	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	3.9	214
322	Modeling solvent effects on electron-spin-resonance hyperfine couplings by frozen-density embedding. *Journal of Chemical Physics*, **2005**, 123, 114101	3.9	57
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320	Photophysics of octabutoxy phthalocyaninato-Ni(II) in toluene: ultrafast experiments and DFT/TDDFT studies. *Journal of Physical Chemistry A*, **2005**, 109, 2078-89	2.8	46
319	Away from generalized gradient approximation: orbital-dependent exchange-correlation functionals. *Journal of Chemical Physics*, **2005**, 123, 62202	3.9	50

318	An improved density matrix functional by physically motivated repulsive corrections. *Journal of Chemical Physics*, **2005**, 122, 204102	3.9	158
317	Rotational effects in the dissociative adsorption of H2 on the Pt211 stepped surface. *Journal of Chemical Physics*, **2005**, 123, 164702	3.9	20
316	Importance of vibronic effects on the circular dichroism spectrum of dimethyloxirane. *Journal of Chemical Physics*, **2005**, 122, 234305	3.9	52
315	Mechanisms of H2 dissociative adsorption on the Pt(211) stepped surface. *Journal of Chemical Physics*, **2005**, 122, 194708	3.9	57
314	The merits of the frozen-density embedding scheme to model solvatochromic shifts. *Journal of Chemical Physics*, **2005**, 122, 094115	3.9	187
313	The uranyl ion revisited: the electric field gradient at U as a probe of environmental effects. *Molecular Physics*, **2005**, 103, 775-787	1.7	10
312	Vibronic coupling and double excitations in linear response time-dependent density functional calculations: dipole-allowed states of N2. *Journal of Chemical Physics*, **2004**, 121, 6155-66	3.9	71
311	Asymptotic correction of the exchange-correlation kernel of time-dependent density functional theory for long-range charge-transfer excitations. *Journal of Chemical Physics*, **2004**, 121, 655-60	3.9	314
310	Reactive scattering of H2 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, 11379-87	3.9	23
309	Adsorption and diffusion on a stepped surface: atomic hydrogen on Pt(211). *Journal of Chemical Physics*, **2004**, 120, 11852-63	3.9	58
308	The spin-unrestricted molecular Kohn-Sham solution and the analogue of Koopmans's theorem for open-shell molecules. *Journal of Chemical Physics*, **2004**, 120, 8364-72	3.9	75
307	Improving numerical integration through basis set expansion. *Theoretical Chemistry Accounts*, **2004**, 112, 410-418	1.9	4
306	Strongly Nucleophilic RhI Centre in Square-Planar Complexes with Terdentate (Ñ) 2,2?:6?,2??-Terpyridine Ligands: Crystallographic, Electrochemical and Density Functional Theoretical Studies. *European Journal of Inorganic Chemistry*, **2004**, 2004, 1675-1686	2.3	19
305	Hydrogen bonding in mimics of Watson-Crick base pairs involving C-H proton donor and F proton acceptor groups: a theoretical study. *ChemPhysChem*, **2004**, 5, 481-7	3.2	41
304	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	3.5	782
303	Even-tempered Slater-type orbitals revisited: from hydrogen to krypton. *Journal of Computational Chemistry*, **2004**, 25, 1030-6	3.5	165
302	How molecular trapping enhances the reactivity of rough surfaces. *Surface Science*, **2004**, 571, L325-L330	1.8	24
301	Dissociative chemisorption of H2 on Pt(111): isotope effect and effects of the rotational distribution and energy dispersion. *Surface Science*, **2004**, 573, 433-445	1.8	39

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298	Improved Description of Chemical Barriers with Generalized Gradient Approximations (GGAs) and Meta-GGAs. *Journal of Physical Chemistry A*, **2004**, 108, 4459-4469	2.8	46
297	Calculation of the A term of magnetic circular dichroism based on time dependent-density functional theory I. Formulation and implementation. *Journal of Chemical Physics*, **2004**, 120, 10942-54	3.9	50
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295	Excitation Energies of Metal Complexes with Time-dependent Density Functional Theory. *Structure and Bonding*, **2004**, 49-116	0.9	69
294	Methane-to-methanol oxidation by the hydrated iron(IV) oxo species in aqueous solution: a combined DFT and car-parrinello molecular dynamics study. *Journal of the American Chemical Society*, **2004**, 126, 4355-65	16.4	97
293	The rotation barrier in ethane. *Nachrichten Aus Der Chemie*, **2004**, 52, 581-581	0.1	4
292	CO on Pt(111): A puzzle revisited. *Journal of Chemical Physics*, **2003**, 119, 4522-4528	3.9	92
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290	STO and GTO field-induced polarization functions for H to Kr. *Journal of Computational Chemistry*, **2003**, 24, 1582-91	3.5	21
289	O2 Evolution in the Fenton Reaction.. *ChemInform*, **2003**, 34, no		1
288	Fenton-Like Chemistry in Water: Oxidation Catalysis by Fe(III) and H2O2.. *ChemInform*, **2003**, 34, no		3
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286	The case for steric repulsion causing the staggered conformation of ethane. *Angewandte Chemie - International Edition*, **2003**, 42, 4183-8; discussion 4188-94	16.4	204
285	Fenton-like Chemistry in Water: Oxidation Catalysis by Fe(III) and H2O2. *Journal of Physical Chemistry A*, **2003**, 107, 5722-5731	2.8	158
284	Photodissociation of the phosphine-substituted transition metal carbonyl complexes Cr(CO)(5)L and Fe(CO)(4)L: a theoretical study. *Journal of the American Chemical Society*, **2003**, 125, 3558-67	16.4	31
283	Effects of Porphyrin Core Saddling, meso-Phenyl Twisting, and Counterions on the Optical Properties of meso-Tetraphenylporphyrin Diacids: The [H4TPP](X)2 (X = F, Cl, Br, I) Series as a Case Study. *Journal of Physical Chemistry A*, **2003**, 107, 11468-11482	2.8	122

282	Nuclear magnetic resonance chemical shifts with the statistical average of orbital-dependent model potentials in Kohn Sham density functional theory. *Journal of Chemical Physics*, **2003**, 118, 8584-8593	3.9	46
281	Exchange-correlation energy and potential as approximate functionals of occupied and virtual Kohn Sham orbitals: Application to dissociating H[sub 2]. *Journal of Chemical Physics*, **2003**, 118, 7183	3.9	47
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279	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	3.9	30
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277	DFT calculations on the electronic and geometrical structure of 18-crown-6 complexes with Ag+, Hg2+, Ag0, Hg+, Hg0, AgNO3, and HgX2 (X=Cl, Br, and I). *Computational and Theoretical Chemistry*, **2002**, 588, 55-69		39
276	A least squares multicenter approach to continuum wave functions. *Chemical Physics*, **2002**, 284, 565-574	2.3	3
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274	Variational density matrix functional calculations for the corrected Hartree and corrected Hartree Bock functionals. *Chemical Physics Letters*, **2002**, 364, 409-419	2.5	49
273	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	3.9	107
272	Dissociative and diffractive scattering of H2 from Pt(111): A four-dimensional quantum dynamics study. *Journal of Chemical Physics*, **2002**, 116, 9435-9448	3.9	28
271	Signatures of site-specific reaction of H2 on Cu(100). *Journal of Chemical Physics*, **2002**, 117, 6673-6687	3.9	33
270	On the required shape corrections to the local density and generalized gradient approximations to the Kohn Sham potentials for molecular response calculations of (hyper)polarizabilities and excitation energies. *Journal of Chemical Physics*, **2002**, 116, 9591-9601	3.9	111
269	Exchange potential from the common energy denominator approximation for the Kohn Sham Green function: Application to (hyper)polarizabilities of molecular chains. *Journal of Chemical Physics*, **2002**, 116, 6435-6442	3.9	87
268	Response Properties of Furan Homologues by Time-Dependent Density Functional Theory. *Journal of Physical Chemistry A*, **2002**, 106, 10380-10390	2.8	9
267	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	3.5	49
266	Electronic structure, chemical bond, and optical spectra of metal bis(porphyrin) complexes: a DFT/TDDFT study of the bis(porphyrin)M(IV) (M = Zr, Ce, Th) series. *Journal of the American Chemical Society*, **2002**, 124, 12319-34	16.4	54
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