Evert Jan Baerends

List of Publications by Citations

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	Chemistry with ADF. *Journal of Computational Chemistry*, **2001**, 22, 931-967	3.5	7628
424	Relativistic regular two-component Hamiltonians. *Journal of Chemical Physics*, **1993**, 99, 4597-4610	3.9	3229
423	Self-consistent molecular Hartree–Fock–Slater calculations I. The computational procedure. *Chemical Physics*, **1973**, 2, 41-51	2.3	2841
422	Relativistic total energy using regular approximations. *Journal of Chemical Physics*, **1994**, 101, 9783-9792	3.9	2379
421	Towards an order-. *Theoretical Chemistry Accounts*, **1998**, 99, 391	1.9	2259
420	Geometry optimizations in the zero order regular approximation for relativistic effects. *Journal of Chemical Physics*, **1999**, 110, 8943-8953	3.9	1855
419	Optimized Slater-type basis sets for the elements 1-118. *Journal of Computational Chemistry*, **2003**, 24, 1142-56	3.5	1780
418	The zero-order regular approximation for relativistic effects: The effect of spin–orbit coupling in closed shell molecules. *Journal of Chemical Physics*, **1996**, 105, 6505-6516	3.9	1273
417	Exchange-correlation potential with correct asymptotic behavior. *Physical Review A*, **1994**, 49, 2421-2431	2.6	1247
416	Towards an order-N DFT method. *Theoretical Chemistry Accounts*, **1998**, 99, 391-403	1.9	1110
415	Relativistic regular two-component Hamiltonians. *International Journal of Quantum Chemistry*, **1996**, 57, 281-293	2.1	923
414	On the calculation of multiplet energies by the hartree-fock-slater method. *Theoretica Chimica Acta*, **1977**, 43, 261-271		830
413	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
412	Three-dimensional numerical integration for electronic structure calculations. *International Journal of Quantum Chemistry*, **1988**, 33, 87-113	2.1	679
411	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	3.9	646
410	Implementation of time-dependent density functional response equations. *Computer Physics Communications*, **1999**, 118, 119-138	4.2	561
409	A Quantum Chemical View of Density Functional Theory. *Journal of Physical Chemistry A*, **1997**, 101, 5383-5403	2.8	511

408	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	16.4	479
407	Assessment of Conventional Density Functional Schemes for Computing the Dipole Moment and (Hyper)polarizabilities of Push−Pull π-Conjugated Systems. *Journal of Physical Chemistry A*, **2000**, 104, 4755-4763	2.8	473
406	Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry. *Reviews in Computational Chemistry*, **2007**, 1-86		466
405	Interpretation of the Kohn−Sham orbital energies as approximate vertical ionization potentials. *Journal of Chemical Physics*, **2002**, 116, 1760-1772	3.9	433
404	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	3.9	429
403	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	3.9	406
402	Self-consistent molecular Hartree−Fock−Slater calculations II. The effect of exchange scaling in some small molecules. *Chemical Physics*, **1973**, 2, 52-59	2.3	405
401	Precise density-functional method for periodic structures. *Physical Review B*, **1991**, 44, 7888-7903	3.3	391
400	Approximation of the exchange-correlation Kohn−Sham potential with a statistical average of different orbital model potentials. *Chemical Physics Letters*, **1999**, 302, 199-207	2.5	390
399	Hydrogen Bonding in DNA Base Pairs: Reconciliation of Theory and Experiment. *Journal of the American Chemical Society*, **2000**, 122, 4117-4128	16.4	379
398	Binding energy and electronic structure of small copper particles. *Physical Review B*, **1983**, 27, 2132-2144	3.3	348
397	Chiroptical properties from time-dependent density functional theory. I. Circular dichroism spectra of organic molecules. *Journal of Chemical Physics*, **2002**, 116, 6930-6940	3.9	346
396	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	3.9	328
395	Electric Field Dependence of the Exchange-Correlation Potential in Molecular Chains. *Physical Review Letters*, **1999**, 83, 694-697	7.4	326
394	Calculation of bond energies in compounds of heavy elements by a quasi-relativistic approach. *The Journal of Physical Chemistry*, **1989**, 93, 3050-3056		325
393	A perturbation theory approach to relativistic calculations. *Molecular Physics*, **1979**, 38, 1909-1929	1.7	318
392	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
391	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	4.8	303

390	A density functional theory study of frequency-dependent polarizabilities and Van der Waals dispersion coefficients for polyatomic molecules. *Journal of Chemical Physics*, **1995**, 103, 9347-9354	3.9	301
389	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	16.4	299
388	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
387	A DFT/TDDFT interpretation of the ground and excited states of porphyrin and porphyrazine complexes. *Coordination Chemistry Reviews*, **2002**, 230, 5-27	23.2	273
386	The Carbon□lithium Electron Pair Bond in (CH3Li)n (n = 1, 2, 4). *Organometallics*, **1996**, 15, 2923-2931	3.8	249
385	Relativistic effects on bonding. *Journal of Chemical Physics*, **1981**, 74, 1271-1284	3.9	241
384	Density-functional-theory response-property calculations with accurate exchange-correlation potentials. *Physical Review A*, **1998**, 57, 2556-2571	2.6	231
383	Ground State of the (H2O)2+ Radical Cation: DFT versus Post-Hartree□ock Methods. *Journal of Physical Chemistry A*, **1999**, 103, 166-170	2.8	223
382	An approximate exchange-correlation hole density as a functional of the natural orbitals. *Molecular Physics*, **2002**, 100, 401-421	1.7	219
381	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
380	Self-consistent approximation to the Kohn-Sham exchange potential. *Physical Review A*, **1995**, 51, 1944-1954	2.6	209
379	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
378	The merits of the frozen-density embedding scheme to model solvatochromic shifts. *Journal of Chemical Physics*, **2005**, 122, 094115	3.9	187
377	Improved density functional theory results for frequency-dependent polarizabilities, by the use of an exchange-correlation potential with correct asymptotic behavior. *Journal of Chemical Physics*, **1996**, 105, 3142-3151	3.9	184
376	Calculating frequency-dependent hyperpolarizabilities using time-dependent density functional theory. *Journal of Chemical Physics*, **1998**, 109, 10644-10656	3.9	181
375	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	2.8	180
374	Time-dependent Density Functional Results for the Dynamic Hyperpolarizability of C60. *Physical Review Letters*, **1997**, 78, 3097-3100	7.4	178
373	Exchange and correlation energy in density functional theory: Comparison of accurate density functional theory quantities with traditional Hartree□ock based ones and generalized gradient approximations for the molecules Li2, N2, F2. *Journal of Chemical Physics*, **1997**, 107, 5007-5015	3.9	177

372	Atomic and molecular hydrogen interacting with Pt(111). *Journal of Chemical Physics*, **1999**, 111, 11155-11163	3.9	176
371	Cohesive energy of 3d transition metals: Density functional theory atomic and bulk calculations. *Physical Review B*, **1996**, 54, 5326-5333	3.3	175
370	Reactive and nonreactive scattering of H2 from a metal surface is electronically adiabatic. *Science*, **2006**, 312, 86-9	33.3	173
369	Predicting catalysis: understanding ammonia synthesis from first-principles calculations. *Journal of Physical Chemistry B*, **2006**, 110, 17719-35	3.4	168
368	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	3.9	168
367	Alternatives to the CO Ligand: Coordination of the Isolobal Analogues BF, BNH2, BN(CH3)2, and BO□In Mono- and Binuclear First-Row Transition Metal Complexes. *Chemistry - A European Journal*, **1998**, 4, 210-221	4.8	165
366	Even-tempered Slater-type orbitals revisited: from hydrogen to krypton. *Journal of Computational Chemistry*, **2004**, 25, 1030-6	3.5	165
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362	Time-dependent density functional calculations on the electronic absorption spectrum of free base porphin. *Journal of Chemical Physics*, **1999**, 111, 2499-2506	3.9	158
361	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
360	Accurate density functional calculations on frequency-dependent hyperpolarizabilities of small molecules. *Journal of Chemical Physics*, **1998**, 109, 10657-10668	3.9	155
359	Quantum theory of dissociative chemisorption on metal surfaces. *Accounts of Chemical Research*, **2002**, 35, 193-200	24.3	154
358	A Density Functional Study of the MLCT States of [Ru(bpy)3]2+ in D3 Symmetry. *Inorganic Chemistry* , **1994**, 33, 3538-3543	5.1	151
357	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	150
356	Comparison of the Accurate Kohn□Sham Solution with the Generalized Gradient Approximations (GGAs) for the SN2 Reaction F- + CH3F -iFCH3 + F-: A Qualitative Rule To Predict Success or Failure of GGAs. *Journal of Physical Chemistry A*, **2000**, 104, 8558-8565	2.8	147
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353	Metal-Macrocycle Interaction in Phthalocyanines: Density Functional Calculations of Ground and Excited States. *Inorganic Chemistry*, **1994**, 33, 584-595	5.1	144
352	The Mechanism of Zinc(II)-Dithiocarbamate-Accelerated Vulcanization Uncovered; Theoretical and Experimental Evidence. *Journal of the American Chemical Society*, **1999**, 121, 163-168	16.4	142
351	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
350	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	139
349	Can the Counterpoise Correction for Basis Set Superposition Effect Be Justified?. *Journal of Chemical Theory and Computation*, **2014**, 10, 252-67	6.4	134
348	Exact solutions of regular approximate relativistic wave equations for hydrogen-like atoms. *Journal of Chemical Physics*, **1994**, 101, 1272-1281	3.9	131
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346	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	3.9	127
345	Self-consistent molecular Hartree-Fock-Slater calculations. *Chemical Physics*, **1975**, 8, 412-418	2.3	126
344	Ethylene epoxidation on silver(110): the role of subsurface oxygen. *The Journal of Physical Chemistry*, **1989**, 93, 6469-6475		125
343	Relativistic atomic orbital contractions and expansions: magnitudes and explanations. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1990**, 23, 3225-3240	1.3	125
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339	DFT study of the active intermediate in the Fenton reaction. *Chemistry - A European Journal*, **2001**, 7, 2775-83	4.8	121
338	The ZORA formalism applied to the Dirac-Fock equation. *Chemical Physics Letters*, **1995**, 246, 632-640	2.5	121
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336	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
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333	Basis Set Effects in Density Functional Calculations on the Metal□igand and Metal□Metal Bonds of Cr(CO)5□□O and (CO)5Mn□Mn(CO)5. *The Journal of Physical Chemistry*, **1996**, 100, 5690-5696		115
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330	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
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325	Nucleophilic or electrophilic phosphinidene complexes ML(n)=PH; what makes the difference?. *Journal of the American Chemical Society*, **2002**, 124, 2831-8	16.4	109
324	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
323	An analytical six-dimensional potential energy surface for dissociation of molecular hydrogen on Cu(100). *Journal of Chemical Physics*, **1996**, 104, 7344-7358	3.9	106
322	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	101
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304	Cr□CO Photodissociation in Cr(CO)6: Reassessment of the Role of Ligand-Field Excited States in the Photochemical Dissociation of Metal□ligand Bonds. *Journal of the American Chemical Society*, **1997**, 119, 7324-7329	16.4	82
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302	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
301	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	16.4	81

300	A Car-Parrinello study of the formation of oxidizing intermediates from Fenton's reagent in aqueous solution. *Physical Chemistry Chemical Physics*, **2002**, 4, 3619-3627	3.6	79
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