Vicenzo Barone

List of Publications by Citations

783 papers	73,105 citations	93 h-index	255 g-index
812 ext. papers	78,965 ext. citations	4.8 avg, IF	8.31 L-index

#	Paper	IF	Citations
783	Toward reliable density functional methods without adjustable parameters: The PBE0 model. *Journal of Chemical Physics*, **1999**, 110, 6158-6170	3.9	11214
782	Quantum Calculation of Molecular Energies and Energy Gradients in Solution by a Conductor Solvent Model. *Journal of Physical Chemistry A*, **1998**, 102, 1995-2001	2.8	6761
781	Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model. *Journal of Computational Chemistry*, **2003**, 24, 669-81	3.5	5805
780	Ab initio study of solvated molecules: a new implementation of the polarizable continuum model. *Chemical Physics Letters*, **1996**, 255, 327-335	2.5	2731
779	Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. *Journal of Chemical Physics*, **1998**, 108, 664-675	3.9	2722
778	A new definition of cavities for the computation of solvation free energies by the polarizable continuum model. *Journal of Chemical Physics*, **1997**, 107, 3210-3221	3.9	2065
777	New developments in the polarizable continuum model for quantum mechanical and classical calculations on molecules in solution. *Journal of Chemical Physics*, **2002**, 117, 43-54	3.9	2048
776	Time-dependent density functional theory for molecules in liquid solutions. *Journal of Chemical Physics*, **2001**, 115, 4708-4717	3.9	1663
775	Geometry optimization of molecular structures in solution by the polarizable continuum model. *Journal of Computational Chemistry*, **1998**, 19, 404-417	3.5	1446
774	Ab initio study of ionic solutions by a polarizable continuum dielectric model. *Chemical Physics Letters*, **1998**, 286, 253-260	2.5	1350
773	Anharmonic vibrational properties by a fully automated second-order perturbative approach. *Journal of Chemical Physics*, **2005**, 122, 14108	3.9	1183
772	Geometries and properties of excited states in the gas phase and in solution: theory and application of a time-dependent density functional theory polarizable continuum model. *Journal of Chemical Physics*, **2006**, 124, 94107	3.9	989
771	Accurate excitation energies from time-dependent density functional theory: Assessing the PBE0 model. *Journal of Chemical Physics*, **1999**, 111, 2889-2899	3.9	592
770	A state-specific polarizable continuum model time dependent density functional theory method for excited state calculations in solution. *Journal of Chemical Physics*, **2006**, 125, 054103	3.9	586
769	Role and effective treatment of dispersive forces in materials: Polyethylene and graphite crystals as test cases. *Journal of Computational Chemistry*, **2009**, 30, 934-9	3.5	549
768	Vibrational zero-point energies and thermodynamic functions beyond the harmonic approximation. *Journal of Chemical Physics*, **2004**, 120, 3059-65	3.9	455
767	Effective method for the computation of optical spectra of large molecules at finite temperature including the Duschinsky and Herzberg-Teller effect: the Qx band of porphyrin as a case study. *Journal of Chemical Physics*, **2008**, 128, 224311	3.9	418

766	Effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution. *Journal of Chemical Physics*, **2007**, 126, 084509	3.9	398
765	Toward effective and reliable fluorescence energies in solution by a new state specific polarizable continuum model time dependent density functional theory approach. *Journal of Chemical Physics*, **2007**, 127, 074504	3.9	384
764	Recent Advances in the Description of Solvent Effects with the Polarizable Continuum Model. *Advances in Quantum Chemistry*, **1998**, 32, 227-261	1.4	373
763	Solvent effect on vertical electronic transitions by the polarizable continuum model. *Journal of Chemical Physics*, **2000**, 112, 2427-2435	3.9	358
762	Fully Integrated Approach to Compute Vibrationally Resolved Optical Spectra: From Small Molecules to Macrosystems. *Journal of Chemical Theory and Computation*, **2009**, 5, 540-54	6.4	353
761	Transverse polarisation of quarks in hadrons. *Physics Reports*, **2002**, 359, 1-168	27.7	343
760	Singlet excited-state behavior of uracil and thymine in aqueous solution: a combined experimental and computational study of 11 uracil derivatives. *Journal of the American Chemical Society*, **2006**, 128, 607-19	16.4	336
759	Fully anharmonic IR and Raman spectra of medium-size molecular systems: accuracy and interpretation. *Physical Chemistry Chemical Physics*, **2014**, 16, 1759-87	3.6	308
758	Interplay of electronic, environmental, and vibrational effects in determining the hyperfine coupling constants of organic free radicals. *Chemical Reviews*, **2004**, 104, 1231-54	68.1	298
757	Polarizable dielectric model of solvation with inclusion of charge penetration effects. *Journal of Chemical Physics*, **2001**, 114, 5691-5701	3.9	284
756	Effective method to compute vibrationally resolved optical spectra of large molecules at finite temperature in the gas phase and in solution. *Journal of Chemical Physics*, **2007**, 126, 184102	3.9	271
755	A second-order perturbation theory route to vibrational averages and transition properties of molecules: general formulation and application to infrared and vibrational circular dichroism spectroscopies. *Journal of Chemical Physics*, **2012**, 136, 124108	3.9	266
754	Magnetic coupling in biradicals, binuclear complexes and wide-gap insulators: a survey of ab initio wave function and density functional theory approaches. *Theoretical Chemistry Accounts*, **2000**, 104, 265-272	1.9	253
753	General Time Dependent Approach to Vibronic Spectroscopy Including Franck-Condon, Herzberg-Teller, and Duschinsky Effects. *Journal of Chemical Theory and Computation*, **2013**, 9, 4097-115	6.4	235
752	Toward chemical accuracy in the computation of NMR shieldings: the PBE0 model. *Chemical Physics Letters*, **1998**, 298, 113-119	2.5	226
751	General Approach to Compute Vibrationally Resolved One-Photon Electronic Spectra. *Journal of Chemical Theory and Computation*, **2010**, 6, 1256-1274	6.4	225
750	Harmonic and Anharmonic Vibrational Frequency Calculations with the Double-Hybrid B2PLYP Method: Analytic Second Derivatives and Benchmark Studies. *Journal of Chemical Theory and Computation*, **2010**, 6, 2115-25	6.4	220
749	Spin density in a nitronyl nitroxide free radical. Polarized neutron diffraction investigation and ab initio calculations. *Journal of the American Chemical Society*, **1994**, 116, 2019-2027	16.4	207

748	Density Functional Calculations of Magnetic Exchange Interactions in Polynuclear Transition Metal Complexes. *Inorganic Chemistry*, **1997**, 36, 5022-5030	5.1	203
747	Analytical second derivatives of the free energy in solution by polarizable continuum models. *Journal of Chemical Physics*, **1998**, 109, 6246-6254	3.9	203
746	General Perturbative Approach for Spectroscopy, Thermodynamics, and Kinetics: Methodological Background and Benchmark Studies. *Journal of Chemical Theory and Computation*, **2012**, 8, 1015-36	6.4	202
745	Development and Validation of the B3LYP/N07D Computational Model for Structural Parameter and Magnetic Tensors of Large Free Radicals. *Journal of Chemical Theory and Computation*, **2008**, 4, 751-64	6.4	202
744	Proton transfer in the ground and lowest excited states of malonaldehyde: A comparative density functional and post-Hartree□Fock study. *Journal of Chemical Physics*, **1996**, 105, 11007-11019	3.9	201
743	A TDDFT study of the electronic spectrum of s-tetrazine in the gas-phase and in aqueous solution. *Chemical Physics Letters*, **2000**, 330, 152-160	2.5	186
742	Prediction of the pKa of Carboxylic Acids Using the ab Initio Continuum-Solvation Model PCM-UAHF. *Journal of Physical Chemistry A*, **1998**, 102, 6706-6712	2.8	185
741	Development and validation of reliable quantum mechanical approaches for the study of free radicals in solution. *Journal of Chemical Physics*, **1996**, 105, 11060-11067	3.9	182
740	Conformation of pleionomers of .alpha.-aminoisobutyric acid. *Macromolecules*, **1985**, 18, 895-902	5.5	178
739	Absorption and fluorescence spectra of uracil in the gas phase and in aqueous solution: a TD-DFT quantum mechanical study. *Journal of the American Chemical Society*, **2004**, 126, 14320-1	16.4	172
738	Absolute pKa determination for carboxylic acids using density functional theory and the polarizable continuum model. *Chemical Physics Letters*, **2003**, 373, 411-415	2.5	168
737	Vibrational computations beyond the harmonic approximation: performances of the B3LYP density functional for semirigid molecules. *Journal of Computational Chemistry*, **2005**, 26, 384-8	3.5	168
736	A Theoretical Investigation of the Ground and Excited States of Selected Ru and Os Polypyridyl Molecular Dyes. *Journal of Physical Chemistry A*, **2002**, 106, 11354-11360	2.8	166
735	Conformational behavior of gaseous glycine by a density functional approach. *Journal of Chemical Physics*, **1995**, 102, 364-370	3.9	162
734	Ab initio calculations of absorption spectra of large molecules in solution: coumarin C153. *Angewandte Chemie - International Edition*, **2007**, 46, 405-8	16.4	157
733	Separation between Fast and Slow Polarizations in Continuum Solvation Models. *Journal of Physical Chemistry A*, **2000**, 104, 10614-10622	2.8	157
732	On the Calculation and Modeling of Magnetic Exchange Interactions in Weakly Bonded Systems: The Case of the Ferromagnetic Copper(II) &mgr;(2)-Azido Bridged Complexes. *Inorganic Chemistry*, **1999**, 38, 1996-2004	5.1	154
731	Hydrogen and higher shell contributions in Zn2+, Ni2+, and Co2+ aqueous solutions: an X-ray absorption fine structure and molecular dynamics study. *Journal of the American Chemical Society*, **2002**, 124, 1958-67	16.4	153

730	On the performance of continuum solvation methods. A comment on "Universal approaches to solvation modeling". *Accounts of Chemical Research*, **2009**, 42, 489-92; discussion 493-7	24.3	152
729	Integrated computational strategies for UV/vis spectra of large molecules in solution. *Chemical Society Reviews*, **2007**, 36, 1724-31	58.5	151
728	Structure, Magnetic Properties and Reactivities of Open-Shell Species From Density Functional and Self-Consistent Hybrid Methods. *Recent Advances in Computational*, **1995**, 287-334		146
727	Quantum mechanical computations and spectroscopy: from small rigid molecules in the gas phase to large flexible molecules in solution. *Accounts of Chemical Research*, **2008**, 41, 605-16	24.3	142
726	Solvent effect on the singlet excited-state lifetimes of nucleic acid bases: A computational study of 5-fluorouracil and uracil in acetonitrile and water. *Journal of the American Chemical Society*, **2006**, 128, 16312-22	16.4	142
725	Transverse-spin and transverse-momentum effects in high-energy processes. *Progress in Particle and Nuclear Physics*, **2010**, 65, 267-333	10.6	140
724	A direct procedure for the evaluation of solvent effects in MC-SCF calculations. *Journal of Chemical Physics*, **1999**, 111, 5295-5302	3.9	140
723	Inclusion of HartreeBock exchange in density functional methods. Hyperfine structure of second row atoms and hydrides. *Journal of Chemical Physics*, **1994**, 101, 6834-6838	3.9	139
722	Validation of self-consistent hybrid density functionals for the study of structural and electronic characteristics of organic radicals. *Journal of Chemical Physics*, **1995**, 102, 384-393	3.9	133
721	Accurate Vibrational Spectra of Large Molecules by Density Functional Computations beyond the Harmonic Approximation:´ The Case of Azabenzenes. *Journal of Physical Chemistry A*, **2004**, 108, 4146-4150	2.8	131
720	Polarizable Force Fields and Polarizable Continuum Model: A Fluctuating Charges/PCM Approach. 1. Theory and Implementation. *Journal of Chemical Theory and Computation*, **2011**, 7, 3711-24	6.4	126
719	Inexpensive and accurate predictions of optical excitations in transition-metal complexes: the TDDFT/PBE0 route. *Theoretical Chemistry Accounts*, **2000**, 105, 169-172	1.9	126
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717	Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments. *Physical Chemistry Chemical Physics*, **2012**, 14, 12404-22	3.6	122
716	Influence of base stacking on excited-state behavior of polyadenine in water, based on time-dependent density functional calculations. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 9931-6	11.5	119
715	Physically motivated density functionals with improved performances: The modified PerdewBurkeErnzerhof model. *Journal of Chemical Physics*, **2002**, 116, 5933-5940	3.9	119
714	A fully automated implementation of VPT2 Infrared intensities. *Chemical Physics Letters*, **2010**, 496, 157-161	1.9	118
713	Structural revision of clusianone and 7-epi-clusianone and anti-HIV activity of polyisoprenylated benzophenones. *Tetrahedron*, **2005**, 61, 8206-8211	2.4	116

712	Structure and conformational behavior of biopolymers by density functional calculations employing periodic boundary conditions. I. The case of polyglycine, polyalanine, and poly-alpha-aminoisobutyric acid in vacuo. *Journal of the American Chemical Society*, **2001**, 123, 3311-22	16.4	115
711	Achieving linear-scaling computational cost for the polarizable continuum model of solvation. *Theoretical Chemistry Accounts*, **2004**, 111, 90-100	1.9	112
710	Accurate Harmonic/Anharmonic Vibrational Frequencies for Open-Shell Systems: Performances of the B3LYP/N07D Model for Semirigid Free Radicals Benchmarked by CCSD(T) Computations. *Journal of Chemical Theory and Computation*, **2010**, 6, 828-38	6.4	109
709	Integrated computational approach to vibrationally resolved electronic spectra: anisole as a test case. *Journal of Chemical Physics*, **2008**, 128, 244105	3.9	109
708	Accurate and feasible computations of structural and magnetic properties of large free radicals: The PBE0/N07D model. *Chemical Physics Letters*, **2008**, 454, 139-143	2.5	107
707	Accurate excitation energies from time-dependent density functional theory: assessing the PBE0 model for organic free radicals. *Chemical Physics Letters*, **1999**, 314, 152-157	2.5	106
706	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. *Chemical Reviews*, **2019**, 119, 8131-8191	68.1	103
705	Gas-phase formation of the prebiotic molecule formamide: insights from new quantum computations. *Monthly Notices of the Royal Astronomical Society: Letters*, **2015**, 453, L31-L35	4.3	103
704	Accurate structure, thermodynamic and spectroscopic parameters from CC and CC/DFT schemes: the challenge of the conformational equilibrium in glycine. *Physical Chemistry Chemical Physics*, **2013**, 15, 10094-111	3.6	102
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701	Linear Response Theory and Electronic Transition Energies for a Fully Polarizable QM/Classical Hamiltonian. *Journal of Chemical Theory and Computation*, **2012**, 8, 4153-65	6.4	100
700	Excited states decay of the A-T DNA: A PCM/TD-DFT study in aqueous solution of the (9-methyl-adenine)(2).(1-methyl-thymine)(2) stacked tetramer. *Journal of the American Chemical Society*, **2009**, 131, 15232-45	16.4	99
699	Accurate vibrational spectra of large molecules by density functional computations beyond the harmonic approximation: the case of uracil and 2-thiouracil. *Chemical Physics Letters*, **2004**, 388, 279-283	2.5	99
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697	Extending the molecular size in accurate quantum-chemical calculations: the equilibrium structure and spectroscopic properties of uracil. *Physical Chemistry Chemical Physics*, **2011**, 13, 7189-97	3.6	97
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695	Conformational characterization of lanthanide(III)-DOTA complexes by ab initio investigation in vacuo and in aqueous solution. *Journal of the American Chemical Society*, **2002**, 124, 4901-9	16.4	97

694	Accurate Anharmonic Vibrational Frequencies for Uracil: The Performance of Composite Schemes and Hybrid CC/DFT Model. *Journal of Chemical Theory and Computation*, **2011**, 7, 3702-10	6.4	96
693	Vibrational spectra of large molecules by density functional computations beyond the harmonic approximation: the case of pyrrole and furan. *Chemical Physics Letters*, **2004**, 383, 528-532	2.5	96
692	Assessment of a Combined QM/MM Approach for the Study of Large Nitroxide Systems in Vacuo and in Condensed Phases. *Journal of the American Chemical Society*, **1998**, 120, 7069-7078	16.4	94
691	Density Functional Study of Intrinsic and Environmental Effects in the Tautomeric Equilibrium of 2-Pyridone. *The Journal of Physical Chemistry*, **1995**, 99, 15062-15068		94
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688	Checking the pH-induced conformational transition of prion protein by molecular dynamics simulations: effect of protonation of histidine residues. *Biophysical Journal*, **2004**, 87, 3623-32	2.9	88
687	Hydrogen-bonding effects on infrared spectra from anharmonic computations: uracil-water complexes and uracil dimers. *Journal of Physical Chemistry A*, **2015**, 119, 4224-36	2.8	87
686	Characterization of the potential energy surface of the HO2 molecular system by a density functional approach. *Journal of Chemical Physics*, **1994**, 101, 10666-10676	3.9	87
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677	Accurate static polarizabilities by density functional theory: assessment of the PBE0 model. *Chemical Physics Letters*, **1999**, 307, 265-271	2.5	82

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671	Intrinsic and Environmental Effects in the Structure and Magnetic Properties of Glycine Radical in Aqueous Solution. *Journal of the American Chemical Society*, **1997**, 119, 12962-12967	16.4	79
670	Quantum mechanical study of the conformational behavior of proline and 4R-hydroxyproline dipeptide analogues in vacuum and in aqueous solution. *Journal of Computational Chemistry*, **2002**, 23, 341-50	3.5	79
669	Performances of different density functionals in the computation of vibrational spectra beyond the harmonic approximation. *Chemical Physics Letters*, **2004**, 399, 226-229	2.5	77
668	Solvent Polarity and pH Effects on the Magnetic Properties of Ionizable Nitroxide Radicals: A Combined Computational and Experimental Study of 2,2,5,5-Tetramethyl-3-carboxypyrrolidine and 2,2,6,6-Tetramethyl-4-carboxypiperidine Nitroxides. *Journal of Physical Chemistry A*, **2002**, 106, 10700-10706	2.8	77
667	Dispersion corrected DFT approaches for anharmonic vibrational frequency calculations: nucleobases and their dimers. *Physical Chemistry Chemical Physics*, **2014**, 16, 10112-28	3.6	76
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665	Reliable NMR chemical shifts for molecules in solution by methods rooted in density functional theory. *Magnetic Resonance in Chemistry*, **2004**, 42 Spec no, S57-67	2.1	76
664	Inclusion of Hartree-Fock exchange in the density functional approach. Benchmark computations for diatomic molecules containing H, B, C, N, O, and F atoms. *Chemical Physics Letters*, **1994**, 226, 392-398	2.5	76
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656	A hybrid explicit/implicit solvation method for first-principle molecular dynamics simulations. *Journal of Chemical Physics*, **2008**, 128, 144501	3.9	72
655	The role of dispersion correction to DFT for modelling weakly bound molecular complexes in the ground and excited electronic states. *Chemical Physics*, **2008**, 346, 247-256	2.3	72
654	Conformational behavior of □dialkylated peptides. *Biopolymers*, **1985**, 24, 1759-1767	2.2	72
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644	Structural versatility of peptides from C□dialkylated glycines. II. An IR absorption and 1H-nmr study of homo-oligopeptides from C□diethylglycine. *Biopolymers*, **1988**, 27, 373-379	2.2	67
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642	Absorption and Emission Spectra of a Flexible Dye in Solution: a Computational Time-Dependent Approach. *Journal of Chemical Theory and Computation*, **2013**, 9, 4507-4516	6.4	66
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