Giovanni Scalmani

List of Publications by Year
in descending order

85 papers	17,909 citations	71102 41 h-index	53230 85 g-index
85 all docs	85 docs citations	85 times ranked	17592 citing authors

#	Article	IF	Citations
1	Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model. Journal of Computational Chemistry, 2003, 24, 669-681.	3.3	6,758
2	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.	3.0	2,235
3	Continuous surface charge polarizable continuum models of solvation. I. General formalism. Journal of Chemical Physics, 2010, 132, 114110.	3.0	2,116
4	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, 094107.	3.0	1,143
5	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.	3.0	675
6	Formation and relaxation of excited states in solution: A new time dependent polarizable continuum model based on time dependent density functional theory. Journal of Chemical Physics, 2006, 124, 124520.	3.0	484
7	Singlet Excited-State Behavior of Uracil and Thymine in Aqueous Solution:Â A Combined Experimental and Computational Study of 11 Uracil Derivatives. Journal of the American Chemical Society, 2006, 128, 607-619.	13.7	359
8	Polarizable dielectric model of solvation with inclusion of charge penetration effects. Journal of Chemical Physics, 2001, 114, 5691-5701.	3.0	315
9	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. Journal of Chemical Physics, 2007, 126, 144105.	3.0	290
10	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, 2115-2125.	5.3	274
11	Practical computation of electronic excitation in solution: vertical excitation model. Chemical Science, 2011, 2, 2143.	7.4	202
12	A TD-DFT investigation of ground and excited state properties in indoline dyes used for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2009, 11, 11276.	2.8	161
13	First hyperpolarizability of polymethineimine with long-range corrected functionals. Journal of Chemical Physics, 2007, 126, 191108.	3.0	158
14	Achieving linear-scaling computational cost for the polarizable continuum model of solvation. Theoretical Chemistry Accounts, 2004, 111, 90-100.	1.4	120
15	Time-dependent density functional theory investigation of the absorption, fluorescence, and phosphorescence spectra of solvated coumarins. Journal of Chemical Physics, 2006, 125, 164324.	3.0	115
16	Time-Dependent Density Functional Tight Binding: New Formulation and Benchmark of Excited States. Journal of Chemical Theory and Computation, 2011, 7, 3304-3313.	5.3	105
17	Accurate static polarizabilities by density functional theory: assessment of the PBE0 model. Chemical Physics Letters, 1999, 307, 265-271.	2.6	86
18	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, 341-350.	3.3	81

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19	Studies of the Ground and Excited-State Surfaces of the Retinal Chromophore using CAM-B3LYP. Journal of Physical Chemistry B, 2010, 114, 5547-5555.	2.6	79
20	A New Approach to Noncollinear Spin Density Functional Theory beyond the Local Density Approximation. Journal of Chemical Theory and Computation, 2012, 8, 2193-2196.	5.3	79
21	Absorption and emission spectra in gas-phase and solution using TD-DFT: Formaldehyde and benzene as case studies. Chemical Physics Letters, 2006, 421, 272-276.	2.6	70
22	Analytical First and Second Derivatives for a Fully Polarizable QM/Classical Hamiltonian. Journal of Chemical Theory and Computation, 2012, 8, 4270-4278.	5.3	68
23	Two-Component Noncollinear Time-Dependent Spin Density Functional Theory for Excited State Calculations. Journal of Chemical Theory and Computation, 2017, 13, 2591-2603.	5.3	66
24	Ground State Properties of the Nucleic Acid Constituents Studied by Density Functional Calculations. I. Conformational Features of Ribose, Dimethyl Phosphate, Uridine, Cytidine, 5â€˜-Methyl Phosphateâ€™Uridine, and 3â€˜-Methyl Phosphateâ€™Uridine. Journal of Physical Chemistry A, 1999, 103, 8716-8724.	2.5	65
25	How the Environment Controls Absorption and Fluorescence Spectra of PRODAN:â€‰ A Quantum-Mechanical Study in Homogeneous and Heterogeneous Media. Journal of Physical Chemistry B, 2008, 112, 414-423.	2.6	65
26	A Single Chiroptical Spectroscopic Method May Not Be Able To Establish the Absolute Configurations of Diastereomers: Dimethylesters of Hibiscus and Garcinia Acids. Journal of Physical Chemistry A, 2011, 115, 5665-5673.	2.5	65
27	The geometries, absorption and fluorescence wavelengths of solvated fluorescent coumarins: A CIS and TD-DFT comparative study. Chemical Physics Letters, 2007, 438, 208-212.	2.6	63
28	Noncollinear density functional theory having proper invariance and local torque properties. Physical Review B, 2013, 87, .	3.2	60
29	On the structure of polaronic defects in thiophene oligomers: a combined Hartreeâ€“Fock and Density Functional Theory study. Synthetic Metals, 2000, 108, 165-172.	3.9	59
30	Absorption and emission spectra of 1,8-naphthalimide fluorophores: A PCM-TD-DFT investigation. Chemical Physics, 2010, 372, 61-66.	1.9	58
31	Radical cations of DNA bases: some insights on structure and fragmentation patterns by density functional methods. International Journal of Mass Spectrometry, 2000, 201, 321-336.	1.5	57
32	On the Calculation of Vibrational Frequencies for Molecules in Solution Beyond the Harmonic Approximation. Journal of Chemical Theory and Computation, 2010, 6, 1660-1669.	5.3	52
33	Accurate Excited-State Geometries: A CASPT2 and Coupled-Cluster Reference Database for Small Molecules. Journal of Chemical Theory and Computation, 2017, 13, 6237-6252.	5.3	52
34	Vertical Electronic Excitations in Solution with the EOM-CCSD Method Combined with a Polarizable Explicit/Implicit Solvent Model. Journal of Chemical Theory and Computation, 2013, 9, 3035-3042.	5.3	48
35	Quantum, classical, and hybrid QM/MM calculations in solution: General implementation of the ddCOSMO linear scaling strategy. Journal of Chemical Physics, 2014, 141, 184108.	3.0	47
36	Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. Chemical Science, 2019, 10, 7200-7211.	7.4	45

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37	Structure and Stereochemical Determination of Hypogeamicins from a Cave-Derived Actinomycete. Journal of Natural Products, 2014, 77, 1759-1763.	3.0	44
38	Charge transfer excitations in TDDFT: A ghostâ€hunter index. Journal of Computational Chemistry, 2017, 38, 2151-2156.	3.3	44
39	Fluorescence of 1,8-naphthalimide: A PCM-TD-DFT investigation. Chemical Physics Letters, 2007, 448, 3-6.	2.6	43
40	Computational Spectroscopy of Large Systems in Solution: The DFTB/PCM and TD-DFTB/PCM Approach. Journal of Chemical Theory and Computation, 2013, 9, 2052-2071.	5.3	43
41	Double hybrids and timeâ€dependent density functional theory: An implementation and benchmark on charge transfer excited states. Journal of Computational Chemistry, 2020, 41, 1242-1251.	3.3	42
42	Coupled Cluster Calculations in Solution with the Polarizable Continuum Model of Solvation. Journal of Physical Chemistry Letters, 2010, 1, 2369-2373.	4.6	41
43	Computation of the acetone ultraviolet spectrum in gas phase and in aqueous solution by a mixed discrete/continuum model. Molecular Physics, 2003, 101, 1945-1953.	1.7	39
44	Polarizable Embedding Approach for the Analytical Calculation of Raman and Raman Optical Activity Spectra of Solvated Systems. Journal of Chemical Theory and Computation, 2017, 13, 4421-4435.	5.3	39
45	Solvation of Coumarin 153 in Supercritical Fluoroform. Journal of Physical Chemistry B, 2006, 110, 4953-4962.	2.6	38
46	Simple Protocol for Capturing Both Linear-Response and State-Specific Effects in Excited-State Calculations with Continuum Solvation Models. Journal of Chemical Theory and Computation, 2021, 17, 5155-5164.	5.3	36
47	Practical Density Functionals beyond the Overdelocalizationâ€“Underbinding Zero-Sum Game. Journal of Physical Chemistry Letters, 2017, 8, 4314-4318.	4.6	35
48	Excited State Dipole Moments in Solution: Comparison between State-Specific and Linear-Response TD-DFT Values. Journal of Chemical Theory and Computation, 2018, 14, 1544-1553.	5.3	33
49	How far do electrons delocalize?. Journal of Chemical Physics, 2014, 141, 144104.	3.0	32
50	Quantum Calculations in Solution for Large to Very Large Molecules: A New Linear Scaling QM/Continuum Approach. Journal of Physical Chemistry Letters, 2014, 5, 953-958.	4.6	32
51	Self-Consistent Field and Polarizable Continuum Model: A New Strategy of Solution for the Coupled Equations. Journal of Chemical Theory and Computation, 2011, 7, 610-617.	5.3	31
52	Comparative Study of Nonhybrid Density Functional Approximations for the Prediction of 3d Transition Metal Thermochemistry. Journal of Chemical Theory and Computation, 2017, 13, 4907-4913.	5.3	30
53	Non covalent interactions in RNA and DNA base pairs: a quantum-mechanical study of the coupling between solvent and electronic density. Physical Chemistry Chemical Physics, 2009, 11, 11617.	2.8	27
54	Excited state gradients for a state-specific continuum solvation approach: The vertical excitation model within a Lagrangian TDDFT formulation. Journal of Chemical Physics, 2017, 146, 204106.	3.0	26

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55	Environmental effects on electronic absorption spectra using DFT: An organic and positively charged fused polycyclic chromophore as a case study. Computational and Theoretical Chemistry, 2009, 914, 94-99.	1.5	24
56	Density-Dependent Formulation of Dispersionâ€“Repulsion Interactions in Hybrid Multiscale Quantum/Molecular Mechanics (QM/MM) Models. Journal of Chemical Theory and Computation, 2018, 14, 1671-1681.	5.3	24
57	M11plus: A Range-Separated Hybrid Meta Functional with Both Local and Rung-3.5 Correlation Terms and High Across-the-Board Accuracy for Chemical Applications. Journal of Chemical Theory and Computation, 2019, 15, 4804-4815.	5.3	24
58	Practical auxiliary basis implementation of Rung 3.5 functionals. Journal of Chemical Physics, 2014, 141, 034103.	3.0	23
59	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. Journal of Chemical Theory and Computation, 2017, 13, 2789-2803.	5.3	23
60	Interplay of Intrinsic and Environmental Effects on the Magnetic Properties of Free Radicals Issuing from H-Atom Addition to Cytosine. Journal of the American Chemical Society, 2001, 123, 7113-7117.	13.7	22
61	Quantifying solvated electrons' delocalization. Physical Chemistry Chemical Physics, 2015, 17, 18305-18317.	2.8	22
62	How are the charge transfer descriptors affected by the quality of the underpinning electronic density?. Journal of Computational Chemistry, 2018, 39, 735-742.	3.3	22
63	Assessing challenging intraâ€•and <scp>interâ€molecular chargeâ€transfer</scp> excitations energies with <scp>doubleâ€hybrid</scp> density functionals. Journal of Computational Chemistry, 2021, 42, 970-981.	3.3	22
64	On the structure of bipolaronic defects in thiophene oligomers: a density functional study. Synthetic Metals, 1998, 92, 69-73.	3.9	21
65	Brueckner doubles coupled cluster method with the polarizable continuum model of solvation. Journal of Chemical Physics, 2011, 134, 244113.	3.0	19
66	Investigating the optical properties of BOIMPY dyes using ab initio tools. Physical Chemistry Chemical Physics, 2017, 19, 10554-10561.	2.8	19
67	Theoretical Study of a New Building Block for Organic Conductors:Â Tetrathiapentalene and Its Radical Cation. Journal of Physical Chemistry B, 1999, 103, 6863-6869.	2.6	18
68	Excited-State Vibrations of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2015, 11, 847-850.	5.3	18
69	Long-range-corrected Rung 3.5 density functional approximations. Journal of Chemical Physics, 2018, 148, 104112.	3.0	18
70	Use of molecular symmetry in the computation of solvation energies and their analytical derivatives by the polarizable continuum model. Chemical Physics Letters, 1999, 301, 263-269.	2.6	17
71	How to make continuum solvation incredibly fast in a few simple steps: A practical guide to the domain decomposition paradigm for the conductorâ€like screening model. International Journal of Quantum Chemistry, 2019, 119, e25669.	2.0	17
72	Quantifying Electron Delocalization in Electrides. Journal of Chemical Theory and Computation, 2016, 12, 79-91.	5.3	15

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73	Analytic second derivatives for semiempirical models based on MNDO. Molecular Physics, 2009, 107, 881-887.	1.7	14
74	Theoretical investigation of the electronic and optical properties of oligothiophenes upon methyl, thiol, and thiomethyl substitutions. Polymer, 2006, 47, 6692-6697.	3.8	13
75	Electronic Couplings for Resonance Energy Transfer from CCSD Calculations: From Isolated to Solvated Systems. Journal of Chemical Theory and Computation, 2015, 11, 5219-5228.	5.3	12
76	Electron Delocalization Range in Atoms and on Molecular Surfaces. Journal of Chemical Theory and Computation, 2016, 12, 3185-3194.	5.3	11
77	Quantum Calculations in Solution of Energies, Structures, and Properties with a Domain Decomposition Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2019, 15, 6061-6073.	5.3	11
78	M11plus, a Range-Separated Hybrid Meta Functional Incorporating Nonlocal Rung-3.5 Correlation, Exhibits Broad Accuracy on Diverse Databases. Journal of Physical Chemistry Letters, 2020, 11, 3045-3050.	4.6	10
79	On the Importance of the Orbital Relaxation in Ground-State Coupled Cluster Calculations in Solution with the Polarizable Continuum Model of Solvation. Journal of Chemical Theory and Computation, 2011, 7, 4012-4018.	5.3	9
80	Structure and stability of spheroalkanes (CH)10. Computational and Theoretical Chemistry, 1995, 338, 31-41.	1.5	8
81	Density functionals for nondynamical correlation constructed from an upper bound to the exact exchange energy density. Molecular Physics, 2019, 117, 1226-1241.	1.7	8
82	Exact-Two-Component Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 2947-2954.	5.3	7
83	Molecular Dynamics Simulations Enforcing Nonperiodic Boundary Conditions: New Developments and Application to the Solvent Shifts of Nitroxide Magnetic Parameters. Journal of Chemical Theory and Computation, 2022, , .	5.3	5
84	Ab initio calculation of stereoelectronic properties of syn-blocked bithiophenes as a tool for the interpretation of conductivity differences in derived doped polymers. Computational and Theoretical Chemistry, 1996, 366, 43-53.	1.5	2
85	Calculation of magnetic properties with density functional approximations including rung 3.5 ingredients. Journal of Chemical Physics, 2020, 153, 164101.	3.0	1