

Giovanni Scalmani

List of Publications by Year in descending order

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85
papers

17,909
citations

81434

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60403

85
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docs citations

85
times ranked

19612
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Dynamics Simulations Enforcing Nonperiodic Boundary Conditions: New Developments and Application to the Solvent Shifts of Nitroxide Magnetic Parameters. <i>Journal of Chemical Theory and Computation</i> , 2022, , .	2.3	5
2	Exact-Two-Component Multiconfiguration Pair-Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2947-2954.	2.3	7
3	Assessing challenging intra- and intermolecular charge-transfer excitations energies with double-hybrid density functionals. <i>Journal of Computational Chemistry</i> , 2021, 42, 970-981.	1.5	22
4	Simple Protocol for Capturing Both Linear-Response and State-Specific Effects in Excited-State Calculations with Continuum Solvation Models. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5155-5164.	2.3	36
5	Calculation of magnetic properties with density functional approximations including rung 3.5 ingredients. <i>Journal of Chemical Physics</i> , 2020, 153, 164101.	1.2	1
6	M11plus, a Range-Separated Hybrid Meta Functional Incorporating Nonlocal Rung-3.5 Correlation, Exhibits Broad Accuracy on Diverse Databases. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3045-3050.	2.1	10
7	Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states. <i>Journal of Computational Chemistry</i> , 2020, 41, 1242-1251.	1.5	42
8	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. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4804-4815.	2.3	24
9	Quantum Calculations in Solution of Energies, Structures, and Properties with a Domain Decomposition Polarizable Continuum Model. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6061-6073.	2.3	11
10	Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. <i>Chemical Science</i> , 2019, 10, 7200-7211.	3.7	45
11	How to make continuum solvation incredibly fast in a few simple steps: A practical guide to the domain decomposition paradigm for the conductor-like screening model. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25669.	1.0	17
12	Density functionals for nondynamical correlation constructed from an upper bound to the exact exchange energy density. <i>Molecular Physics</i> , 2019, 117, 1226-1241.	0.8	8
13	Long-range-corrected Rung 3.5 density functional approximations. <i>Journal of Chemical Physics</i> , 2018, 148, 104112.	1.2	18
14	Density-Dependent Formulation of Dispersion-Repulsion Interactions in Hybrid Multiscale Quantum/Molecular Mechanics (QM/MM) Models. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1671-1681.	2.3	24
15	Excited State Dipole Moments in Solution: Comparison between State-Specific and Linear-Response TD-DFT Values. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1544-1553.	2.3	33
16	How are the charge transfer descriptors affected by the quality of the underpinning electronic density?. <i>Journal of Computational Chemistry</i> , 2018, 39, 735-742.	1.5	22
17	Two-Component Noncollinear Time-Dependent Spin Density Functional Theory for Excited State Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2591-2603.	2.3	66
18	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2789-2803.	2.3	23

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19	Excited state gradients for a state-specific continuum solvation approach: The vertical excitation model within a Lagrangian TDDFT formulation. <i>Journal of Chemical Physics</i> , 2017, 146, 204106.	1.2	26
20	Investigating the optical properties of BOIMPY dyes using ab initio tools. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10554-10561.	1.3	19
21	Practical Density Functionals beyond the Overdelocalizationâ€“Underbinding Zero-Sum Game. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4314-4318.	2.1	35
22	Comparative Study of Nonhybrid Density Functional Approximations for the Prediction of 3d Transition Metal Thermochemistry. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4907-4913.	2.3	30
23	Polarizable Embedding Approach for the Analytical Calculation of Raman and Raman Optical Activity Spectra of Solvated Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4421-4435.	2.3	39
24	Charge transfer excitations in TDDFT: A ghostâ€“hunter index. <i>Journal of Computational Chemistry</i> , 2017, 38, 2151-2156.	1.5	44
25	Accurate Excited-State Geometries: A CASPT2 and Coupled-Cluster Reference Database for Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6237-6252.	2.3	52
26	Electron Delocalization Range in Atoms and on Molecular Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3185-3194.	2.3	11
27	Quantifying Electron Delocalization in Electrides. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 79-91.	2.3	15
28	Quantifying solvated electrons' delocalization. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 18305-18317.	1.3	22
29	Excited-State Vibrations of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 847-850.	2.3	18
30	Electronic Couplings for Resonance Energy Transfer from CCSD Calculations: From Isolated to Solvated Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5219-5228.	2.3	12
31	Practical auxiliary basis implementation of Rung 3.5 functionals. <i>Journal of Chemical Physics</i> , 2014, 141, 034103.	1.2	23
32	How far do electrons delocalize?. <i>Journal of Chemical Physics</i> , 2014, 141, 144104.	1.2	32
33	Structure and Stereochemical Determination of Hypogeamicins from a Cave-Derived Actinomycete. <i>Journal of Natural Products</i> , 2014, 77, 1759-1763.	1.5	44
34	Quantum Calculations in Solution for Large to Very Large Molecules: A New Linear Scaling QM/Continuum Approach. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 953-958.	2.1	32
35	Quantum, classical, and hybrid QM/MM calculations in solution: General implementation of the ddCOSMO linear scaling strategy. <i>Journal of Chemical Physics</i> , 2014, 141, 184108.	1.2	47
36	Noncollinear density functional theory having proper invariance and local torque properties. <i>Physical Review B</i> , 2013, 87, .	1.1	60

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37	Computational Spectroscopy of Large Systems in Solution: The DFTB/PCM and TD-DFTB/PCM Approach. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2052-2071.	2.3	43
38	Vertical Electronic Excitations in Solution with the EOM-CCSD Method Combined with a Polarizable Explicit/Implicit Solvent Model. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3035-3042.	2.3	48
39	A New Approach to Noncollinear Spin Density Functional Theory beyond the Local Density Approximation. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2193-2196.	2.3	79
40	Analytical First and Second Derivatives for a Fully Polarizable QM/Classical Hamiltonian. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4270-4278.	2.3	68
41	A Single Chiroptical Spectroscopic Method May Not Be Able To Establish the Absolute Configurations of Diastereomers: Dimethylesters of Hibiscus and Garcinia Acids. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5665-5673.	1.1	65
42	Time-Dependent Density Functional Tight Binding: New Formulation and Benchmark of Excited States. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3304-3313.	2.3	105
43	Self-Consistent Field and Polarizable Continuum Model: A New Strategy of Solution for the Coupled Equations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 610-617.	2.3	31
44	On the Importance of the Orbital Relaxation in Ground-State Coupled Cluster Calculations in Solution with the Polarizable Continuum Model of Solvation. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4012-4018.	2.3	9
45	Practical computation of electronic excitation in solution: vertical excitation model. <i>Chemical Science</i> , 2011, 2, 2143.	3.7	202
46	Brueckner doubles coupled cluster method with the polarizable continuum model of solvation. <i>Journal of Chemical Physics</i> , 2011, 134, 244113.	1.2	19
47	Absorption and emission spectra of 1,8-naphthalimide fluorophores: A PCM-TD-DFT investigation. <i>Chemical Physics</i> , 2010, 372, 61-66.	0.9	58
48	Continuous surface charge polarizable continuum models of solvation. I. General formalism. <i>Journal of Chemical Physics</i> , 2010, 132, 114110.	1.2	2,116
49	Studies of the Ground and Excited-State Surfaces of the Retinal Chromophore using CAM-B3LYP. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5547-5555.	1.2	79
50	On the Calculation of Vibrational Frequencies for Molecules in Solution Beyond the Harmonic Approximation. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1660-1669.	2.3	52
51	Harmonic and Anharmonic Vibrational Frequency Calculations with the Double-Hybrid B2PLYP Method: Analytic Second Derivatives and Benchmark Studies. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2115-2125.	2.3	274
52	Coupled Cluster Calculations in Solution with the Polarizable Continuum Model of Solvation. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2369-2373.	2.1	41
53	Environmental effects on electronic absorption spectra using DFT: An organic and positively charged fused polycyclic chromophore as a case study. <i>Computational and Theoretical Chemistry</i> , 2009, 914, 94-99.	1.5	24
54	A TD-DFT investigation of ground and excited state properties in indoline dyes used for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11276.	1.3	161

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55	Non covalent interactions in RNA and DNA base pairs: a quantum-mechanical study of the coupling between solvent and electronic density. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11617.	1.3	27
56	Analytic second derivatives for semiempirical models based on MNDO. <i>Molecular Physics</i> , 2009, 107, 881-887.	0.8	14
57	How the Environment Controls Absorption and Fluorescence Spectra of PRODAN: A Quantum-Mechanical Study in Homogeneous and Heterogeneous Media. <i>Journal of Physical Chemistry B</i> , 2008, 112, 414-423.	1.2	65
58	First hyperpolarizability of polymethineimine with long-range corrected functionals. <i>Journal of Chemical Physics</i> , 2007, 126, 191108.	1.2	158
59	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. <i>Journal of Chemical Physics</i> , 2007, 126, 144105.	1.2	290
60	The geometries, absorption and fluorescence wavelengths of solvated fluorescent coumarins: A CIS and TD-DFT comparative study. <i>Chemical Physics Letters</i> , 2007, 438, 208-212.	1.2	63
61	Fluorescence of 1,8-naphthalimide: A PCM-TD-DFT investigation. <i>Chemical Physics Letters</i> , 2007, 448, 3-6.	1.2	43
62	Formation and relaxation of excited states in solution: A new time dependent polarizable continuum model based on time dependent density functional theory. <i>Journal of Chemical Physics</i> , 2006, 124, 124520.	1.2	484
63	Time-dependent density functional theory investigation of the absorption, fluorescence, and phosphorescence spectra of solvated coumarins. <i>Journal of Chemical Physics</i> , 2006, 125, 164324.	1.2	115
64	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. <i>Journal of Chemical Physics</i> , 2006, 124, 094107.	1.2	1,143
65	Solvation of Coumarin 153 in Supercritical Fluoroform. <i>Journal of Physical Chemistry B</i> , 2006, 110, 4953-4962.	1.2	38
66	A state-specific polarizable continuum model time dependent density functional theory method for excited state calculations in solution. <i>Journal of Chemical Physics</i> , 2006, 125, 054103.	1.2	675
67	Absorption and emission spectra in gas-phase and solution using TD-DFT: Formaldehyde and benzene as case studies. <i>Chemical Physics Letters</i> , 2006, 421, 272-276.	1.2	70
68	Singlet Excited-State Behavior of Uracil and Thymine in Aqueous Solution: A Combined Experimental and Computational Study of 11 Uracil Derivatives. <i>Journal of the American Chemical Society</i> , 2006, 128, 607-619.	6.6	359
69	Theoretical investigation of the electronic and optical properties of oligothiophenes upon methyl, thiol, and thiomethyl substitutions. <i>Polymer</i> , 2006, 47, 6692-6697.	1.8	13
70	Achieving linear-scaling computational cost for the polarizable continuum model of solvation. <i>Theoretical Chemistry Accounts</i> , 2004, 111, 90-100.	0.5	120
71	Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model. <i>Journal of Computational Chemistry</i> , 2003, 24, 669-681.	1.5	6,758
72	Computation of the acetone ultraviolet spectrum in gas phase and in aqueous solution by a mixed discrete/continuum model. <i>Molecular Physics</i> , 2003, 101, 1945-1953.	0.8	39

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73	New developments in the polarizable continuum model for quantum mechanical and classical calculations on molecules in solution. <i>Journal of Chemical Physics</i> , 2002, 117, 43-54.	1.2	2,235
74	Quantum mechanical study of the conformational behavior of proline and 4R-hydroxyproline dipeptide analogues in vacuum and in aqueous solution. <i>Journal of Computational Chemistry</i> , 2002, 23, 341-350.	1.5	81
75	Interplay of Intrinsic and Environmental Effects on the Magnetic Properties of Free Radicals Issuing from H-Atom Addition to Cytosine. <i>Journal of the American Chemical Society</i> , 2001, 123, 7113-7117.	6.6	22
76	Polarizable dielectric model of solvation with inclusion of charge penetration effects. <i>Journal of Chemical Physics</i> , 2001, 114, 5691-5701.	1.2	315
77	Radical cations of DNA bases: some insights on structure and fragmentation patterns by density functional methods. <i>International Journal of Mass Spectrometry</i> , 2000, 201, 321-336.	0.7	57
78	On the structure of polaronic defects in thiophene oligomers: a combined Hartree-Fock and Density Functional Theory study. <i>Synthetic Metals</i> , 2000, 108, 165-172.	2.1	59
79	Use of molecular symmetry in the computation of solvation energies and their analytical derivatives by the polarizable continuum model. <i>Chemical Physics Letters</i> , 1999, 301, 263-269.	1.2	17
80	Accurate static polarizabilities by density functional theory: assessment of the PBE0 model. <i>Chemical Physics Letters</i> , 1999, 307, 265-271.	1.2	86
81	Ground State Properties of the Nucleic Acid Constituents Studied by Density Functional Calculations. I. Conformational Features of Ribose, Dimethyl Phosphate, Uridine, Cytidine, 5-Methyl Phosphate-Uridine, and 3-Methyl Phosphate-Uridine. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8716-8724.	1.1	65
82	Theoretical Study of a New Building Block for Organic Conductors: Tetrathiapentalene and Its Radical Cation. <i>Journal of Physical Chemistry B</i> , 1999, 103, 6863-6869.	1.2	18
83	On the structure of bipolaronic defects in thiophene oligomers: a density functional study. <i>Synthetic Metals</i> , 1998, 92, 69-73.	2.1	21
84	Ab initio calculation of stereoelectronic properties of syn-blocked bithiophenes as a tool for the interpretation of conductivity differences in derived doped polymers. <i>Computational and Theoretical Chemistry</i> , 1996, 366, 43-53.	1.5	2
85	Structure and stability of spheroalkanes (CH) ₁₀ . <i>Computational and Theoretical Chemistry</i> , 1995, 338, 31-41.	1.5	8