

Franco Egidi

List of Publications by Year in descending order

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Version: 2024-02-01

38
papers

1,163
citations

304743

22
h-index

377865

34
g-index

38
all docs

38
docs citations

38
times ranked

887
citing authors

#	ARTICLE	IF	CITATIONS
1	Implementation of a graphical user interface for the virtual multifrequency spectrometer: The VMSâ€Draw tool. <i>Journal of Computational Chemistry</i> , 2015, 36, 321-334.	3.3	84
2	The Optical Rotation of Methyloxirane in Aqueous Solution: A Never Ending Story?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1880-1884.	5.3	76
3	A Robust and Effective Time-Independent Route to the Calculation of Resonance Raman Spectra of Large Molecules in Condensed Phases with the Inclusion of Duschinsky, Herzbergâ€™Teller, Anharmonic, and Environmental Effects. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 346-363.	5.3	71
4	Real time propagation of the exact two component time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2016, 145, 104107.	3.0	71
5	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.	5.3	66
6	Molecular spectroscopy of aqueous solutions: a theoretical perspective. <i>Chemical Society Reviews</i> , 2020, 49, 5664-5677.	38.1	55
7	Direct Atomic-Orbital-Based Relativistic Two-Component Linear Response Method for Calculating Excited-State Fine Structures. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3711-3718.	5.3	51
8	General Strategy for Computing Nonlinear Optical Properties of Large Neutral and Cationic Organic Chromophores in Solution. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3155-3173.	2.6	50
9	Toward an Accurate Modeling of Optical Rotation for Solvated Systems: Anharmonic Vibrational Contributions Coupled to the Polarizable Continuum Model. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 585-597.	5.3	46
10	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.	5.3	39
11	Simulating vertical excitation energies of solvated dyes: From continuum to polarizable discrete modeling. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25684.	2.0	37
12	Stereoelectronic, Vibrational, and Environmental Contributions to Polarizabilities of Large Molecular Systems: A Feasible Anharmonic Protocol. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2456-2464.	5.3	35
13	The consequences of improperly describing oscillator strengths beyond the electric dipole approximation. <i>Journal of Chemical Physics</i> , 2015, 143, 234103.	3.0	34
14	The Electronic Circular Dichroism of Nicotine in Aqueous Solution: A Test Case for Continuum and Mixed Explicit-Continuum Solvation Approaches. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5396-5404.	2.5	33
15	A combined experimental and theoretical study of optical rotatory dispersion for (<i>R</i>)-glycidyl methyl ether in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3644-3655.	2.8	30
16	Theory and algorithms for chiroptical properties and spectroscopies of aqueous systems. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22864-22879.	2.8	29
17	Accurate structure, thermodynamics, and spectroscopy of medium-sized radicals by hybrid coupled cluster/density functional theory approaches: The case of phenyl radical. <i>Journal of Chemical Physics</i> , 2013, 138, 234303.	3.0	28
18	Binding of SARSâ€CoVâ€2 to Cell Receptors: A Tale of Molecular Evolution. <i>ChemBioChem</i> , 2021, 22, 724-732.	2.6	27

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19	Origin invariance in vibrational resonance Raman optical activity. <i>Journal of Chemical Physics</i> , 2015, 142, 174101.	3.0	25
20	A benchmark study of electronic excitation energies, transition moments, and excited-state energy gradients on the nicotine molecule. <i>Journal of Chemical Physics</i> , 2014, 141, 224114.	3.0	23
21	Optical rotatory dispersion of methyloxirane in aqueous solution: assessing the performance of density functional theory in combination with a fully polarizable QM/MM/PCM approach. <i>Optical Materials Express</i> , 2015, 5, 196.	3.0	23
22	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.	5.3	23
23	Development of a Virtual Spectrometer for Chiroptical Spectroscopies: The Case of Nicotine. <i>Chirality</i> , 2013, 25, 701-708.	2.6	22
24	Current development of noncollinear electronic structure theory. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25398.	2.0	22
25	Multilevel Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 791-803.	5.3	21
26	Calculation of Linear and Non-linear Electric Response Properties of Systems in Aqueous Solution: A Polarizable Quantum/Classical Approach with Quantum Repulsion Effects. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6993-7004.	5.3	16
27	Computational simulation of vibrationally resolved spectra for spin-forbidden transitions. <i>Chirality</i> , 2018, 30, 850-865.	2.6	15
28	On the nature of charge-transfer excitations for molecules in aqueous solution: a polarizable QM/MM study. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	14
29	Synthesis and Optical Properties of Imidazole-Based Fluorophores having High Quantum Yields. <i>ChemPlusChem</i> , 2014, 79, 366-370.	2.8	13
30	Relativistic Two-Component Particle-Particle Tamm-Dancoff Approximation. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5379-5384.	5.3	13
31	Vibrational circular dichroism under the quantum magnifying glass: from the electronic flow to the spectroscopic observable. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4224-4239.	2.8	13
32	Tuning of NMR and EPR parameters by vibrational averaging and environmental effects: an integrated computational approach. <i>Molecular Physics</i> , 2013, 111, 1345-1354.	1.7	12
33	Unlocking the power of resonance Raman spectroscopy: The case of amides in aqueous solution. <i>Journal of Molecular Liquids</i> , 2022, 346, 117841.	4.9	12
34	An efficient and robust procedure to calculate absorption spectra of aqueous charged species applied to NO ₂ ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14857-14872.	2.8	11
35	Amide Spectral Fingerprints are Hydrogen Bonding-Mediated. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6200-6207.	4.6	9
36	A polarizable three-layer frozen density embedding/molecular mechanics approach. <i>Journal of Chemical Physics</i> , 2021, 154, 164107.	3.0	7

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37	Low-lying electronic excitations of a water-soluble BODIPY: from the gas phase to the solvated molecule. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	4
38	Computational hints for the simultaneous spectroscopic detection of common contaminants in water. <i>Journal of Molecular Liquids</i> , 2022, 355, 118908.	4.9	3