Franco Egidi

List of Publications by Year
in descending order

38	1,163	304743	377865
papers	citations	22 h-index	34 g-index

38	38	38	887
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Unlocking the power of resonance Raman spectroscopy: The case of amides in aqueous solution. Journal of Molecular Liquids, 2022, 346, 117841.	4.9	12
2	Computational hints for the simultaneous spectroscopic detection of common contaminants in water. Journal of Molecular Liquids, 2022, 355, 118908.	4.9	3
3	Amide Spectral Fingerprints are Hydrogen Bonding-Mediated. Journal of Physical Chemistry Letters, 2022, 13, 6200-6207.	4.6	9
4	Binding of SARSâ€CoVâ€2 to Cell Receptors: A Tale of Molecular Evolution. ChemBioChem, 2021, 22, 724-732.	2.6	27
5	Multilevel Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 791-803.	5.3	21
6	A polarizable three-layer frozen density embedding/molecular mechanics approach. Journal of Chemical Physics, 2021, 154, 164107.	3.0	7
7	An efficient and robust procedure to calculate absorption spectra of aqueous charged species applied to NO₂^{â^’}. Physical Chemistry Chemical Physics, 2021, 23, 14857-14872.	2.8	11
8	Calculation of Linear and Non-linear Electric Response Properties of Systems in Aqueous Solution: A Polarizable Quantum/Classical Approach with Quantum Repulsion Effects. Journal of Chemical Theory and Computation, 2020, 16, 6993-7004.	5.3	16
9	Theory and algorithms for chiroptical properties and spectroscopies of aqueous systems. Physical Chemistry Chemical Physics, 2020, 22, 22864-22879.	2.8	29
10	Molecular spectroscopy of aqueous solutions: a theoretical perspective. Chemical Society Reviews, 2020, 49, 5664-5677.	38.1	55
11	Simulating vertical excitation energies of solvated dyes: From continuum to polarizable discrete modeling. International Journal of Quantum Chemistry, 2019, 119, e25684.	2.0	37
12	Vibrational circular dichroism under the quantum magnifying glass: from the electronic flow to the spectroscopic observable. Physical Chemistry Chemical Physics, 2019, 21, 4224-4239.	2.8	13
13	A combined experimental and theoretical study of optical rotatory dispersion for (R)-glycidyl methyl ether in aqueous solution. Physical Chemistry Chemical Physics, 2019, 21, 3644-3655.	2.8	30
14	Computational simulation of vibrationally resolved spectra for spinâ€forbidden transitions. Chirality, 2018, 30, 850-865.	2.6	15
15	Current development of noncollinear electronic structure theory. International Journal of Quantum Chemistry, 2018, 118, e25398.	2.0	22
16	On the nature of charge-transfer excitations for molecules in aqueous solution: a polarizable QM/MM study. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	14
17	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
18	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

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19	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
20	Real time propagation of the exact two component time-dependent density functional theory. Journal of Chemical Physics, 2016, 145, 104107.	3.0	71
21	Relativistic Two-Component Particleâ€“Particle Tammâ€“Dancoff Approximation. Journal of Chemical Theory and Computation, 2016, 12, 5379-5384.	5.3	13
22	Direct Atomic-Orbital-Based Relativistic Two-Component Linear Response Method for Calculating Excited-State Fine Structures. Journal of Chemical Theory and Computation, 2016, 12, 3711-3718.	5.3	51
23	Low-lying electronic excitations of a water-soluble BODIPY: from the gas phase to the solvated molecule. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	4
24	The consequences of improperly describing oscillator strengths beyond the electric dipole approximation. Journal of Chemical Physics, 2015, 143, 234103.	3.0	34
25	Origin invariance in vibrational resonance Raman optical activity. Journal of Chemical Physics, 2015, 142, 174101.	3.0	25
26	The Electronic Circular Dichroism of Nicotine in Aqueous Solution: A Test Case for Continuum and Mixed Explicit-Continuum Solvation Approaches. Journal of Physical Chemistry A, 2015, 119, 5396-5404.	2.5	33
27	General Strategy for Computing Nonlinear Optical Properties of Large Neutral and Cationic Organic Chromophores in Solution. Journal of Physical Chemistry B, 2015, 119, 3155-3173.	2.6	50
28	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. Optical Materials Express, 2015, 5, 196.	3.0	23
29	Implementation of a graphical user interface for the virtual multifrequency spectrometer: The VMSâ€Draw tool. Journal of Computational Chemistry, 2015, 36, 321-334.	3.3	84
30	A benchmark study of electronic excitation energies, transition moments, and excited-state energy gradients on the nicotine molecule. Journal of Chemical Physics, 2014, 141, 224114.	3.0	23
31	Synthesis and Optical Properties of Imidazoleâ€Based Fluorophores having High Quantum Yields. ChemPlusChem, 2014, 79, 366-370.	2.8	13
32	Stereoelectronic, Vibrational, and Environmental Contributions to Polarizabilities of Large Molecular Systems: A Feasible Anharmonic Protocol. Journal of Chemical Theory and Computation, 2014, 10, 2456-2464.	5.3	35
33	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. Journal of Chemical Theory and Computation, 2014, 10, 346-363.	5.3	71
34	Development of a Virtual Spectrometer for Chiroptical Spectroscopies: The Case of Nicotine. Chirality, 2013, 25, 701-708.	2.6	22
35	The Optical Rotation of Methyloxirane in Aqueous Solution: A Never Ending Story?. Journal of Chemical Theory and Computation, 2013, 9, 1880-1884.	5.3	76
36	Tuning of NMR and EPR parameters by vibrational averaging and environmental effects: an integrated computational approach. Molecular Physics, 2013, 111, 1345-1354.	1.7	12

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37	Accurate structure, thermodynamics, and spectroscopy of medium-sized radicals by hybrid coupled cluster/density functional theory approaches: The case of phenyl radical. Journal of Chemical Physics, 2013, 138, 234303.	3.0	28
38	Toward an Accurate Modeling of Optical Rotation for Solvated Systems: Anharmonic Vibrational Contributions Coupled to the Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2012, 8, 585-597.	5.3	46