

Javier Cerezo

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

50
papers

993
citations

18
h-index

29
g-index

58
ext. papers

1,172
ext. citations

4.1
avg, IF

4.52
L-index

#	Paper	IF	Citations
50	Insights for an Accurate Comparison of Computational Data to Experimental Absorption and Emission Spectra: Beyond the Vertical Transition Approximation. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2072-82	6.4	166
49	First-principle computation of absorption and fluorescence spectra in solution accounting for vibronic structure, temperature effects and solvent inhomogenous broadening. <i>Computational and Theoretical Chemistry</i> , 2014 , 1040-1041, 328-337	2	77
48	Modeling Solvent Broadening on the Vibronic Spectra of a Series of Coumarin Dyes. From Implicit to Explicit Solvent Models. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5810-25	6.4	54
47	Harmonic Models in Cartesian and Internal Coordinates to Simulate the Absorption Spectra of Carotenoids at Finite Temperatures. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4947-58	6.4	47
46	Absorption and emission spectral shapes of a prototype dye in water by combining classical/dynamical and quantum/static approaches. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 5426-38	2.8	45
45	Vibronic Coupling Explains the Different Shape of Electronic Circular Dichroism and of Circularly Polarized Luminescence Spectra of Hexahelicenes. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2799-819	6.4	40
44	How DNA is damaged by external electric fields: selective mutation vs. random degradation. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 8243-6	3.6	30
43	Revisiting Vertical Models To Simulate the Line Shape of Electronic Spectra Adopting Cartesian and Internal Coordinates. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4970-4985	6.4	26
42	Disentangling vibronic and solvent broadening effects in the absorption spectra of coumarin derivatives for dye sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 11401-11	3.6	25
41	Antioxidant properties of Carotene isomers and their role in photosystems: insights from Ab initio simulations. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 3498-506	2.8	25
40	Depth characterization by confocal raman microscopy of oxygen inhibition in free radical photopolymerization of acrylates: Contribution of the thiol chemistry. <i>Journal of Polymer Science Part A</i> , 2013 , 51, 635-643	2.5	24
39	Labelling Herceptin with a novel oxaliplatin derivative: a computational approach towards the selective drug delivery. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2401	2	23
38	Adiabatic-Molecular Dynamics Generalized Vertical Hessian Approach: A Mixed Quantum Classical Method To Compute Electronic Spectra of Flexible Molecules in the Condensed Phase. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 1215-1231	6.4	23
37	Optical Properties of Diarylethenes with TD-DFT: 0-0 Energies, Fluorescence, Stokes Shifts, and Vibronic Shapes. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3944-57	6.4	22
36	Mixed Quantum/Classical Method for Nonadiabatic Quantum Dynamics in Explicit Solvent Models: The π/π^* Decay of Thymine in Water as a Test Case. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 820-832	6.4	20
35	Developing accurate intramolecular force fields for conjugated systems through explicit coupling terms. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	20
34	Counterion-Mediated Crossing of the Cyanine Limit in Crystals and Fluid Solution: Bond Length Alternation and Spectral Broadening Unveiled by Quantum Chemistry. <i>Journal of the American Chemical Society</i> , 2020 , 142, 2835-2843	16.4	19

33	Atomistic molecular dynamics simulations of the interactions of oleic and 2-hydroxyoleic acids with phosphatidylcholine bilayers. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 11727-38	3.4	19
32	Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function. <i>Journal of Chemical Physics</i> , 2020 , 152, 054107	3.9	18
31	Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges. <i>Journal of Chemical Physics</i> , 2019 , 151, 064107	3.9	18
30	Comparing classical approaches with empirical or quantum-mechanically derived force fields for the simulation electronic lineshapes: application to coumarin dyes. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	18
29	A Tris(triphenylphosphine)ruthenium(II) Complex as a UV Photoinitiator for Free-Radical Polymerization and in Situ Silver Nanoparticle Formation in Cationic Films. <i>Macromolecules</i> , 2013 , 46, 8808-8815	5.5	17
28	Vibrationally resolved electronic spectra including vibrational pre-excitation: Theory and application to VIPER spectroscopy. <i>Journal of Chemical Physics</i> , 2017 , 147, 164116	3.9	17
27	Conformational changes of β -carotene and zeaxanthin immersed in a model membrane through atomistic molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 6527-38	3.6	17
26	Quantum-Classical Calculation of Vibronic Spectra along a Reaction Path: The Case of the ECD of Easily Interconvertible Conformers with Opposite Chiral Responses. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 4891-4897	6.4	15
25	Multistate coupled quantum dynamics of photoexcited cytosine in gas-phase: Nonadiabatic absorption spectrum and ultrafast internal conversions. <i>Chemical Physics</i> , 2018 , 515, 452-463	2.3	15
24	Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 22889-905	3.6	13
23	Comparative studies on the inhibitory activities of selected benzoic acid derivatives against secretory phospholipase A2, a key enzyme involved in the inflammatory pathway. <i>Molecular BioSystems</i> , 2015 , 11, 1973-9		12
22	Structure, Spectra, and DFT Simulation of Nickel Benzazolate Complexes with Tris(2-aminoethyl)amine Ligand. <i>Inorganic Chemistry</i> , 2017 , 56, 3663-3673	5.1	11
21	Comparison of the results of a mean-field mixed quantum/classical method with full quantum predictions for nonadiabatic dynamics: application to the ($\pi \rightarrow \pi^*$) decay of thymine. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	10
20	Rovibrational energies, partition functions and equilibrium fractionation of the CO2 isotopologues. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2014 , 147, 233-251	2.1	10
19	A computational study of the vibrationally-resolved electronic circular dichroism spectra of single-chain transoid and cisoid oligothiophenes in chiral conformations. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 21864-21880	3.6	9
18	Short- and Long-Range Solvation Effects on the Transient UV-Vis Absorption Spectra of a Ru(II)-Polypyridine Complex Disentangled by Nonequilibrium Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 2885-2891	6.4	8
17	Structure and spectroscopic properties of nickel benzazolate complexes with hydrotris(pyrazolyl)borate ligand. <i>Inorganic Chemistry</i> , 2014 , 53, 5502-14	5.1	8
16	Toward a general mixed quantum/classical method for the calculation of the vibronic ECD of a flexible dye molecule with different stable conformers: Revisiting the case of 2,2,2-trifluoro-anthrylethanol. <i>Chirality</i> , 2018 , 30, 730-743	2.1	7

15	Electronic spectroscopy of a solvatochromic dye in water: comparison of static cluster/implicit and dynamical/explicit solvent models on structures and energies. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	7
14	Accounting for Vibronic Features through a Mixed Quantum-Classical Scheme: Structure, Dynamics, and Absorption Spectra of a Perylene Diimide Dye in Solution. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 7061-7077	6.4	7
13	Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 8181-8199	3.6	7
12	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. <i>ChemPhotoChem</i> , 2019 , 3, 846-855	3.3	6
11	The shape of the electronic circular dichroism spectrum of (2,6-dimethylphenyl)(phenyl)methanol: interplay between conformational equilibria and vibronic effects. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 32349-32360	3.6	6
10	The Intriguing Case of the One-Photon and Two-Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Wave-Function Methods. <i>ChemPhotoChem</i> , 2019 , 3, 778-793	3.3	5
9	Oxygen-Mediated Reactions in Photopolymerizable Radical Thin Films: Application to Simultaneous Photocuring Under Air and Nanoparticle Formation. <i>Macromolecular Chemistry and Physics</i> , 2015 , 216, 1702-1711	2.6	5
8	Energetic Self-Folding Mechanism in α -Helices. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 8186-8194	3.4	3
7	Molecular vibration as a novel explanatory mechanism for the expression of animal colouration. <i>Integrative Biology (United Kingdom)</i> , 2018 , 10, 464-473	3.7	3
6	Theoretical insights on the antioxidant activity of edaravone free radical scavengers derivatives. <i>Chemical Physics Letters</i> , 2014 , 599, 73-79	2.5	3
5	On the Role of Entropy in the Stabilization of α -Helices. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 6523-6531	6.1	2
4	Vibronic approach to the calculation of the decay rate of the photoexcited charge-transfer state of Guanine-Cytosine stacked dimer in water solution. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	2
3	Solvent effect on the energetics of proton coupled electron transfer in guanine-cytosine pair in chloroform by mixed explicit and implicit solvation models. <i>Chemical Physics</i> , 2018 , 515, 493-501	2.3	2
2	Intraresidual Correlated Motions in Peptide Chains. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 4524-4527	6.1	2
1	Partition Functions and Thermodynamic Quantities for the Molecular Hydrogen Isotopologues. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 9226-9241	2.8	1