Javier Cerezo

List of Publications by Year in Descending Order

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	Partition Functions and Thermodynamic Quantities for the Molecular Hydrogen Isotopologues. *Journal of Physical Chemistry A*, **2021**, 125, 9226-9241	2.8	1
49	Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives. *Physical Chemistry Chemical Physics*, **2021**, 23, 8181-8199	3.6	7
48	On the Role of Entropy in the Stabilization of □Helices. *Journal of Chemical Information and Modeling*, **2020**, 60, 6523-6531	6.1	2
47	Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function. *Journal of Chemical Physics*, **2020** , 152, 054107	3.9	18
46	Counterion-Mediated Crossing of the Cyanine Limit in Crystals and Fluid Solution: Bond Length Alternation and Spectral Broadening Unveiled by Quantum Chemistry. *Journal of the American Chemical Society*, **2020**, 142, 2835-2843	16.4	19
45	Adiabatic-Molecular Dynamics Generalized Vertical Hessian Approach: A Mixed Quantum Classical Method To Compute Electronic Spectra of Flexible Molecules in the Condensed Phase. *Journal of Chemical Theory and Computation*, **2020**, 16, 1215-1231	6.4	23
44	Accounting for Vibronic Features through a Mixed Quantum-Classical Scheme: Structure, Dynamics, and Absorption Spectra of a Perylene Diimide Dye in Solution. *Journal of Chemical Theory and Computation*, **2020**, 16, 7061-7077	6.4	7
43	Energetic Self-Folding Mechanism in □Helices. *Journal of Physical Chemistry B*, **2019**, 123, 8186-8194	3.4	3
42	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. *ChemPhotoChem*, **2019**, 3, 846-855	3.3	6
41	The Intriguing Case of the One-Photon and Two-Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Wave-Function Methods. *ChemPhotoChem*, **2019**, 3, 778-793	3.3	5
40	Short- and Long-Range Solvation Effects on the Transient UV-Vis Absorption Spectra of a Ru(II)-Polypyridine Complex Disentangled by Nonequilibrium Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 2885-2891	6.4	8
39	Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges. *Journal of Chemical Physics*, **2019**, 151, 064107	3.9	18
38	Intraresidual Correlated Motions in Peptide Chains. *Journal of Chemical Information and Modeling*, **2019**, 59, 4524-4527	6.1	2
37	Comparison of the results of a mean-field mixed quantum/classical method with full quantum predictions for nonadiabatic dynamics: application to the (pi pi ^*/npi ^*) decay of thymine. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	10
36	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. *Chirality*, **2018**, 30, 730-743	2.1	7
35	Molecular vibration as a novel explanatory mechanism for the expression of animal colouration. *Integrative Biology (United Kingdom)*, **2018**, 10, 464-473	3.7	3
34	A computational study of the vibrationally-resolved electronic circular dichroism spectra of single-chain transoid and cisoid oligothiophenes in chiral conformations. *Physical Chemistry Chemical Physics*, **2018**, 20, 21864-21880	3.6	9

33	Solvent effect on the energetics of proton coupled electron transfer in guanine-cytosine pair in chloroform by mixed explicit and implicit solvation models. *Chemical Physics*, **2018**, 515, 493-501	2.3	2
32	Multistate coupled quantum dynamics of photoexcited cytosine in gas-phase: Nonadiabatic absorption spectrum and ultrafast internal conversions. *Chemical Physics*, **2018**, 515, 452-463	2.3	15
31	Mixed Quantum/Classical Method for Nonadiabatic Quantum Dynamics in Explicit Solvent Models: The π/nπ Decay of Thymine in Water as a Test Case. *Journal of Chemical Theory and Computation* , **2018**, 14, 820-832	6.4	20
30	Developing accurate intramolecular force fields for conjugated systems through explicit coupling terms. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	20
29	Structure, Spectra, and DFT Simulation of Nickel Benzazolate Complexes with Tris(2-aminoethyl)amine Ligand. *Inorganic Chemistry*, **2017**, 56, 3663-3673	5.1	11
28	The shape of the electronic circular dichroism spectrum of (2,6-dimethylphenyl)(phenyl)methanol: interplay between conformational equilibria and vibronic effects. *Physical Chemistry Chemical Physics*, **2017**, 19, 32349-32360	3.6	6
27	Vibrationally resolved electronic spectra including vibrational pre-excitation: Theory and application to VIPER spectroscopy. *Journal of Chemical Physics*, **2017**, 147, 164116	3.9	17
26	Vibronic approach to the calculation of the decay rate of the photoexcited charge-transfer state of Guanine□Cytosine stacked dimer in water solution. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	2
25	Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative. *Physical Chemistry Chemical Physics*, **2016**, 18, 22889-905	3.6	13
24	Quantum-Classical Calculation of Vibronic Spectra along a Reaction Path: The Case of the ECD of Easily Interconvertible Conformers with Opposite Chiral Responses. *Journal of Physical Chemistry Letters*, **2016**, 7, 4891-4897	6.4	15
23	Electronic spectroscopy of a solvatochromic dye in water: comparison of static cluster/implicit and dynamical/explicit solvent models on structures and energies. *Theoretical Chemistry Accounts*, **2016** , 135, 1	1.9	7
22	Comparing classical approaches with empirical or quantum-mechanically derived force fields for the simulation electronic lineshapes: application to coumarin dyes. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	18
21	Vibronic Coupling Explains the Different Shape of Electronic Circular Dichroism and of Circularly Polarized Luminescence Spectra of Hexahelicenes. *Journal of Chemical Theory and Computation*, **2016**, 12, 2799-819	6.4	40
20	Revisiting Vertical Models To Simulate the Line Shape of Electronic Spectra Adopting Cartesian and Internal Coordinates. *Journal of Chemical Theory and Computation*, **2016**, 12, 4970-4985	6.4	26
19	Comparative studies on the inhibitory activities of selected benzoic acid derivatives against secretory phospholipase A2, a key enzyme involved in the inflammatory pathway. *Molecular BioSystems*, **2015**, 11, 1973-9		12
18	Disentangling vibronic and solvent broadening effects in the absorption spectra of coumarin derivatives for dye sensitized solar cells. *Physical Chemistry Chemical Physics*, **2015**, 17, 11401-11	3.6	25
17	Absorption and emission spectral shapes of a prototype dye in water by combining classical/dynamical and quantum/static approaches. *Journal of Physical Chemistry A*, **2015**, 119, 5426-38	2.8	45
16	Modeling Solvent Broadening on the Vibronic Spectra of a Series of Coumarin Dyes. From Implicit to Explicit Solvent Models. *Journal of Chemical Theory and Computation*, **2015**, 11, 5810-25	6.4	54

15	Oxygen-Mediated Reactions in Photopolymerizable Radical Thin Films: Application to Simultaneous Photocuring Under Air and Nanoparticle Formation. *Macromolecular Chemistry and Physics*, **2015**, 216, 1702-1711	2.6	5
14	First-principle computation of absorption and fluorescence spectra in solution accounting for vibronic structure, temperature effects and solvent inhomogenous broadening. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 328-337	2	77
13	Optical Properties of Diarylethenes with TD-DFT: 0-0 Energies, Fluorescence, Stokes Shifts, and Vibronic Shapes. *Journal of Chemical Theory and Computation*, **2014**, 10, 3944-57	6.4	22
12	Structure and spectroscopic properties of nickel benzazolate complexes with hydrotris(pyrazolyl)borate ligand. *Inorganic Chemistry*, **2014**, 53, 5502-14	5.1	8
11	How DNA is damaged by external electric fields: selective mutation vs. random degradation. *Physical Chemistry Chemical Physics*, **2014**, 16, 8243-6	3.6	30
10	Labelling Herceptin with a novel oxaliplatin derivative: a computational approach towards the selective drug delivery. *Journal of Molecular Modeling*, **2014**, 20, 2401	2	23
9	Rovibrational energies, partition functions and equilibrium fractionation of the CO2 isotopologues. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2014**, 147, 233-251	2.1	10
8	Theoretical insights on the antioxidant activity of edaravone free radical scavengers derivatives. *Chemical Physics Letters*, **2014**, 599, 73-79	2.5	3
7	Harmonic Models in Cartesian and Internal Coordinates to Simulate the Absorption Spectra of Carotenoids at Finite Temperatures. *Journal of Chemical Theory and Computation*, **2013**, 9, 4947-58	6.4	47
6	A Tris(triphenylphosphine)ruthenium(II) Complex as a UV Photoinitiator for Free-Radical Polymerization and in Situ Silver Nanoparticle Formation in Cationic Films. *Macromolecules*, **2013**, 46, 8808-8815	5.5	17
5	Depth characterization by confocal raman microscopy of oxygen inhibition in free radical photopolymerization of acrylates: Contribution of the thiol chemistry. *Journal of Polymer Science Part A*, **2013**, 51, 635-643	2.5	24
4	Insights for an Accurate Comparison of Computational Data to Experimental Absorption and Emission Spectra: Beyond the Vertical Transition Approximation. *Journal of Chemical Theory and Computation*, **2013**, 9, 2072-82	6.4	166
3	Conformational changes of β-carotene and zeaxanthin immersed in a model membrane through atomistic molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2013**, 15, 6527-38	3.6	17
2	Antioxidant properties of β-carotene isomers and their role in photosystems: insights from Ab initio simulations. *Journal of Physical Chemistry A*, **2012**, 116, 3498-506	2.8	25
1	Atomistic molecular dynamics simulations of the interactions of oleic and 2-hydroxyoleic acids with phosphatidylcholine bilayers. *Journal of Physical Chemistry B*, **2011**, 115, 11727-38	3.4	19