Francisco JosÃ© Avila Ferrer

List of Publications by Year
in descending order

42 papers	1,509 citations	331670 21 h-index	315739 38 g-index
43 all docs	43 docs citations	43 times ranked	1350 citing authors

#	Article	IF	Citations
1	Origin of Chiroptic Amplification in Perylene-Diimide Helicenes. Journal of Physical Chemistry C, 2021, 125, 2554-2564.	3.1	17
2	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.	5.3	50
3	Proving the Dual Electronic Structure of Charged Metal-Molecule Interfaces: Surface-Enhanced Raman Scattering of Cyanide Adsorbed on a Nanostructured Silver Electrode. Journal of Physical Chemistry C, 2020, 124, 17632-17639.	3.1	6
4	Conical intersections and intersystem crossings explain product formation in photochemical reactions of aryl azides. Physical Chemistry Chemical Physics, 2019, 21, 2389-2396.	2.8	23
5	Theoretical Approaches for Modeling the Effect of the Electrode Potential in the SERS Vibrational Wavenumbers of Pyridine Adsorbed on a Charged Silver Surface. Frontiers in Chemistry, 2019, 7, 423.	3.6	13
6	The Intriguing Case of the Oneâ€Photon and Twoâ€Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Waveâ€Function Methods. ChemPhotoChem, 2019, 3, 778-793.	3.0	8
7	An MS-CASPT2 study of the photodecomposition of 4-methoxyphenyl azide: role of internal conversion and intersystem crossing. Physical Chemistry Chemical Physics, 2018, 20, 7764-7771.	2.8	26
8	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 2,2,2â€trifluoroâ€anthrylethanol. Chirality, 2018, 30, 730-743.	2.6	10
9	Charge transfer at the nanoscale and the role of the out-of-plane vibrations in the selection rules of surface-enhanced Raman scattering. Physical Chemistry Chemical Physics, 2018, 20, 29430-29439.	2.8	15
10	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.	2.8	10
11	Comment on â€œElucidation of charge-transfer SERS selection rules by considering the excited state properties and the role of electrode potentialâ€•by M. Mohammadpour, M. H. Khodabandeh, L. Visscher and Z. Jamshidi, Phys. Chem. Chem. Phys., 2017, 19, 7833. Physical Chemistry Chemical Physics, 2017, 19, 27888-27891.	2.8	8
12	Analysis of the Potential Dependent Surface-Enhanced Raman Scattering of p-Aminothiophenol on the Basis of MS-CASPT2 Calculations. Journal of Physical Chemistry C, 2016, 120, 19322-19328.	3.1	18
13	An approach to the electronic structure of molecular junctions with metal clusters of atomic thickness. Physical Chemistry Chemical Physics, 2016, 18, 27179-27184.	2.8	2
14	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.	1.4	7
15	The absorption and emission spectra in solution of oligothiophene-based pushâ€“pull biomarkers: a PCM/TD-DFT vibronic study. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	5
16	Disentangling vibronic and solvent broadening effects in the absorption spectra of coumarin derivatives for dye sensitized solar cells. Physical Chemistry Chemical Physics, 2015, 17, 11401-11411.	2.8	28
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, 5426-5438.	2.5	50
18	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, 5810-5825.	5.3	66

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19	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part II: Solution Phase. ChemPhysChem, 2014, 15, 3246-3257.	2.1	27
20	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.	2.5	88
21	The excited state behavior of cytosine in the gas phase: A TD-DFT study. Computational and Theoretical Chemistry, 2014, 1040-1041, 186-194.	2.5	25
22	Combination of Transient 2D-IR Experiments and Ab Initio Computations Sheds Light on the Formation of the Charge-Transfer State in Photoexcited Carbonyl Carotenoids. Journal of Physical Chemistry B, 2014, 118, 9613-9630.	2.6	17
23	Quantumâ€Classical Calculation of the Absorption and Emission Spectral Shapes of Oligothiophenes at Low and Room Temperature by Firstâ€Principle Calculations. ChemPhysChem, 2014, 15, 3320-3333.	2.1	25
24	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part I: Gas Phase. ChemPhysChem, 2014, 15, 3236-3245.	2.1	16
25	The interplay between neutral exciton and charge transfer states in single-strand polyadenine: a quantum dynamical investigation. Photochemical and Photobiological Sciences, 2013, 12, 1527.	2.9	16
26	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, 4947-4958.	5.3	62
27	Quantum-classical effective-modes dynamics of the Ï€Ï€* â†' nÏ€* decay in 9H-adenine. A quadratic vibronic coupling model. Faraday Discussions, 2013, 163, 223.	3.2	42
28	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, 2072-2082.	5.3	194
29	Duschinsky, Herzbergâ€"Teller, and Multiple Electronic Resonance Interferential Effects in Resonance Raman Spectra and Excitation Profiles. The Case of Pyrene. Journal of Chemical Theory and Computation, 2013, 9, 3597-3611.	5.3	60
30	Vibrationally Resolved Absorption and Emission Spectra of Dithiophene in the Gas Phase and in Solution by First-Principle Quantum Mechanical Calculations. Journal of Chemical Theory and Computation, 2012, 8, 4483-4493.	5.3	66
31	Comparison of vertical and adiabatic harmonic approaches for the calculation of the vibrational structure of electronic spectra. Physical Chemistry Chemical Physics, 2012, 14, 13549.	2.8	189
32	Modelling the effect of the electrode potential on the metalâ€"adsorbate surface states: relevant states in the charge transfer mechanism of SERS. Chemical Communications, 2011, 47, 4210.	4.1	48
33	Comment on â€œMulticonfigurational perturbation theory can predict a false ground stateâ€•by C. Camacho, R. Cimiraglia and H. A. Witek, Phys. Chem. Chem. Phys., 2010, 12, 5058. Physical Chemistry Chemical Physics, 2011, 13, 7230.	2.8	15
34	How the electrode potential controls the selection rules of the charge transfer mechanism of SERS. Chemical Communications, 2011, 47, 4213.	4.1	50
35	Computing the inhomogeneous broadening of electronic transitions in solution: a first-principle quantum mechanical approach. Physical Chemistry Chemical Physics, 2011, 13, 17007.	2.8	89
36	A molecular mechanism for direct generation of nitric oxide, peroxynitrite and superoxide in the reaction of nitroglycerin with a cysteil-cysteine derivative. Theoretical Chemistry Accounts, 2011, 128, 593-599.	1.4	4

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37	Surface-Enhanced Resonant Raman Scattering Of p-Benzosemiquinone Radical Anion. , 2010, , .		0
38	Role of Dimethyl Sulfoxide in the Hydrolytic Peeling of Boron Nitride Nanotubes. Journal of Physical Chemistry C, 2009, 113, 15565-15568.	3.1	8
39	Outstanding Role of Silver Nanoparticles in the Surface-Enhanced Resonance Raman Scattering of p-Benzosemiquinone. Journal of Physical Chemistry C, 2009, 113, 105-108.	3.1	20
40	Photodissociation mechanism of methyl nitrate. A study with the multistate second-order multiconfigurational perturbation theory. Physical Chemistry Chemical Physics, 2009, 11, 2631.	2.8	30
41	Approach to the Atmospheric Chemistry of Methyl Nitrate and Methylperoxy Nitrite. Chemical Mechanisms of Their Formation and Decomposition Reactions in the Gas Phase. Journal of Physical Chemistry A, 2008, 112, 249-255.	2.5	41
42	Photochemistry of Protonated Nitrosamine: Chemical Inertia of NH₂NOH⁺ Versus Reactivity of NH₃NO⁺. Journal of Physical Chemistry A, 2008, 112, 8394-8402.	2.5	12