Aurora MuÃ±oz Losa

List of Publications by Year
in descending order

45 papers	1,559 citations	471061 17 h-index	301761 39 g-index
45 all docs	45 docs citations	45 times ranked	2034 citing authors

#	Article	IF	Citations
1	What is Solvatochromism?. Journal of Physical Chemistry B, 2010, 114, 17128-17135.	1.2	389
2	Electronic Energy Transfer in Condensed Phase Studied by a Polarizable QM/MM Model. Journal of Chemical Theory and Computation, 2009, 5, 1838-1848.	2.3	259
3	Photosynthetic Light-Harvesting Is Tuned by the Heterogeneous Polarizable Environment of the Protein. Journal of the American Chemical Society, 2011, 133, 3078-3084.	6.6	123
4	Fretting about FRET: Failure of the Ideal Dipole Approximation. Biophysical Journal, 2009, 96, 4779-4788.	0.2	118
5	A Subsystem TDDFT Approach for Solvent Screening Effects on Excitation Energy Transfer Couplings. Journal of Chemical Theory and Computation, 2010, 6, 1843-1851.	2.3	77
6	Quantum mechanical methods applied to excitation energy transfer: A comparative analysis on excitation energies and electronic couplings. Journal of Chemical Physics, 2008, 129, 034104.	1.2	54
7	Energy Flow in the Cryptophyte PE545 Antenna Is Directed by Bilin Pigment Conformation. Journal of Physical Chemistry B, 2013, 117, 4263-4273.	1.2	49
8	A theoretical study of solvent effects on the 1(nâ†'Ï€*) electron transition in acrolein. Journal of Chemical Physics, 2004, 121, 3710-3716.	1.2	37
9	UV-Induced Adenine Radicals Induced in DNA A-Tracts: Spectral and Dynamical Characterization. Journal of Physical Chemistry Letters, 2016, 7, 3949-3953.	2.1	35
10	A CASPT2//CASSCF Study of Vertical and Adiabatic Electron Transitions of Acrolein in Water Solution. Journal of Physical Chemistry B, 2007, 111, 9864-9870.	1.2	34
11	Using Molecular Dynamics and Quantum Mechanics Calculations To Model Fluorescence Observables. Journal of Physical Chemistry A, 2011, 115, 3997-4008.	1.1	30
12	Solvent Effects on the Radiative and Nonradiative Decay of a Model of the Rhodopsin Chromophore. Journal of Chemical Theory and Computation, 2011, 7, 4050-4059.	2.3	26
13	Solvent Effects on the Low-Lying Excited States of a Model of Retinal. Journal of Physical Chemistry B, 2006, 110, 18064-18071.	1.2	24
14	Excited State Pathways Leading to Formation of Adenine Dimers. Journal of Physical Chemistry Letters, 2016, 7, 2020-2023.	2.1	24
15	Nonplasmonic Metal Particles as Excitation Energy Transfer Acceptors: an Unexpected Efficiency Revealed by Quantum Mechanics. Journal of Physical Chemistry C, 2009, 113, 16364-16370.	1.5	21
16	Location of conical intersections in solution using a sequential quantum mechanics/molecular dynamics method. Chemical Physics Letters, 2007, 443, 76-81.	1.2	20
17	Theoretical Study of Solvent Effects on the Ground and Low-Lying Excited Free Energy Surfaces of a Pushâ€"Pull Substituted Azobenzene. Journal of Physical Chemistry B, 2014, 118, 12518-12530.	1.2	18
18	Retinal Models: Comparison of Electronic Absorption Spectra in the Gas Phase and in Methanol Solution. Journal of Physical Chemistry B, 2008, 112, 8815-8823.	1.2	16

#	Article	IF	Citations
19	Solvatochromic Shifts on Absorption and Fluorescence Bands of N,N-Dimethylaniline. Journal of Chemical Theory and Computation, 2009, 5, 341-349.	2.3	16
20	Quantum Mechanical Approach to Solvent Effects on the Optical Properties of Metal Nanoparticles and Their Efficiency As Excitation Energy Transfer Acceptors. Journal of Physical Chemistry C, 2010, 114, 1553-1561.	1.5	16
21	A State-Specific PCMâ€“DFT method to include dynamic solvent effects in the calculation of ionization energies: Application to DNA bases. Chemical Physics Letters, 2015, 634, 20-24.	1.2	15
22	Solvent Effects on the Structure and Spectroscopy of the Emitting States of 1-Phenylpyrrole. Journal of Chemical Theory and Computation, 2011, 7, 1850-1857.	2.3	14
23	Simultaneous Solvent and Counterion Effects on the Absorption Properties of a Model of the Rhodopsin Chromophore. Journal of Chemical Theory and Computation, 2013, 9, 1548-1556.	2.3	14
24	Substituent and Solvent Effects on the UVâ€“vis Absorption Spectrum of the Photoactive Yellow Protein Chromophore. Journal of Physical Chemistry A, 2015, 119, 5504-5514.	1.1	13
25	Solvent Effects on Internal Conversions and Intersystem Crossings:Â The Radiationless De-Excitation of Acrolein in Water. Journal of Physical Chemistry B, 2008, 112, 877-884.	1.2	12
26	Solvent Effects on the Absorption Spectra of the para-Coumaric Acid Chromophore in Its Different Protonation Forms. Journal of Chemical Theory and Computation, 2013, 9, 4481-4494.	2.3	12
27	Theoretical Study of the Competition between Intramolecular Hydrogen Bonds and Solvation in the Cys-Asn-Ser Tripeptide. Journal of Physical Chemistry B, 2010, 114, 8961-8970.	1.2	11
28	Theoretical study of the role of solvent Stark effect in electron transitions. Theoretical Chemistry Accounts, 2011, 128, 783-793.	0.5	10
29	Theoretical study of the conformational equilibrium of 1,4-dioxane in gas phase, neat liquid, and dilute aqueous solutions. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	10
30	Solvent effects on de-excitation channels in the p-coumaric acid methyl ester anion, an analogue of the photoactive yellow protein (PYP) chromophore. Physical Chemistry Chemical Physics, 2016, 18, 27476-27485.	1.3	10
31	An ASEP/MD study of liquid chloroform. Computational and Theoretical Chemistry, 2006, 775, 81-86.	1.5	9
32	Correlated ab initio molecular dynamics simulations of the acetoneâ€“carbon dioxide complex: implications for solubility in supercritical CO₂. Molecular Simulation, 2014, 40, 154-159.	0.9	8
33	QM/MM Study of Substituent and Solvent Effects on the Excited State Dynamics of the Photoactive Yellow Protein Chromophore. Journal of Chemical Theory and Computation, 2017, 13, 737-748.	2.3	8
34	Theoretical study of the absorption and emission spectra of the anionic p-coumaric methyl ester in gas phase and in solution. Computational and Theoretical Chemistry, 2014, 1040-1041, 287-294.	1.1	6
35	How Methylation Modifies the Photophysics of the Native All-trans-Retinal Protonated Schiff Base: A CASPT2/MD Study in Gas Phase and in Methanol. Journal of Physical Chemistry A, 2018, 122, 3096-3106.	1.1	6
36	An averaged solvent electrostatic potential/molecular dynamics study of the influence of the electron correlation on the properties of liquid hydrogen fluoride. Computational and Theoretical Chemistry, 2003, 632, 227-234.	1.5	3

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37	Which strategy for molecular probe design? An answer from the integration of spectroscopy and QM modeling. Physical Chemistry Chemical Physics, 2010, 12, 8999.	1.3	3
38	Dual Fluorescence of Fluorazene in Solution: A Computational Study. Journal of Chemical Theory and Computation, 2011, 7, 3694-3701.	2.3	3
39	The optical properties of adenine cation in different oligonucleotides: a PCM/TD-DFT study. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	3
40	Use of the Average Solvent Potential Approach in the Study of Solvent Effects. Advances in Quantum Chemistry, 2010, 59, 59-97.	0.4	2
41	Fretting About FRET: Breakdown of the Ideal Dipole Approximation. Biophysical Journal, 2010, 98, 582a.	0.2	1
42	Modeling Fluorescence Observables, Particularly for FRET Experiments, using Markov Chain Analysis of Molecular Dynamics and Quantum Mechanics Simulations. Biophysical Journal, 2012, 102, 597a.	0.2	0
43	Modeling Fluorescence Observables, Particularly for FRET Experiments, using Markov Chain Analysis of Molecular Dynamics and Quantum Mechanics Simulations. Biophysical Journal, 2013, 104, 683a.	0.2	0
44	Solvent Effects on Radiative and Non-Radiative Excited State Decays. Challenges and Advances in Computational Chemistry and Physics, 2008, , 135-157.	0.6	0
45	Accelerating QM/MM Calculations by Using the Mean Field Approximation. Challenges and Advances in Computational Chemistry and Physics, 2015, , 135-152.	0.6	0