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	The optical properties of adenine cation in different oligonucleotides: a PCM/TD-DFT study. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	3
2	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
3	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
4	Excited State Pathways Leading to Formation of Adenine Dimers. Journal of Physical Chemistry Letters, 2016, 7, 2020-2023.	2.1	24
5	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
6	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
7	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
8	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
9	Accelerating QM/MM Calculations by Using the Mean Field Approximation. Challenges and Advances in Computational Chemistry and Physics, 2015, , 135-152.	0.6	0
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

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19	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
20	Dual Fluorescence of Fluorazene in Solution: A Computational Study. Journal of Chemical Theory and Computation, 2011, 7, 3694-3701.	2.3	3
21	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
22	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
23	Using Molecular Dynamics and Quantum Mechanics Calculations To Model Fluorescence Observables. Journal of Physical Chemistry A, 2011, 115, 3997-4008.	1.1	30
24	Theoretical study of the role of solvent Stark effect in electron transitions. Theoretical Chemistry Accounts, 2011, 128, 783-793.	0.5	10
25	Fretting About FRET: Breakdown of the Ideal Dipole Approximation. Biophysical Journal, 2010, 98, 582a.	0.2	1
26	What is Solvatochromism?. Journal of Physical Chemistry B, 2010, 114, 17128-17135.	1.2	389
27	Use of the Average Solvent Potential Approach in the Study of Solvent Effects. Advances in Quantum Chemistry, 2010, 59, 59-97.	0.4	2
28	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
29	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
30	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
31	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
32	Solvatochromic Shifts on Absorption and Fluorescence Bands of N,N-Dimethylaniline. Journal of Chemical Theory and Computation, 2009, 5, 341-349.	2.3	16
33	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
34	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
35	Fretting about FRET: Failure of the Ideal Dipole Approximation. Biophysical Journal, 2009, 96, 4779-4788.	0.2	118
36	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

#	Article	IF	Citations
37	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
38	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
39	Solvent Effects on Radiative and Non-Radiative Excited State Decays. Challenges and Advances in Computational Chemistry and Physics, 2008, , 135-157.	0.6	0
40	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
41	Location of conical intersections in solution using a sequential quantum mechanics/molecular dynamics method. Chemical Physics Letters, 2007, 443, 76-81.	1.2	20
42	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
43	An ASEP/MD study of liquid chloroform. Computational and Theoretical Chemistry, 2006, 775, 81-86.	1.5	9
44	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
45	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