MarÃ-a Luz SÃ¡nchez Mendoza

List of Publications by Year
in descending order

22 papers	1,614 citations	516215 16 h-index	642321 23 g-index
23 all docs	23 docs citations	23 times ranked	1114 citing authors

#	Article	IF	Citations
1	The Incorporation of Quantum Effects in Enzyme Kinetics Modeling. Accounts of Chemical Research, 2002, 35, 341-349.	7.6	240
2	Optimized Parameters for Scaling Correlation Energy. Journal of Physical Chemistry A, 1999, 103, 3139-3143.	1.1	184
3	Canonical Variational Theory for Enzyme Kinetics with the Protein Mean Force and Multidimensional Quantum Mechanical Tunneling Dynamics. Theory and Application to Liver Alcohol Dehydrogenase. Journal of Physical Chemistry B, 2001, 105, 11326-11340.	1.2	184
4	Quantum Dynamics of Hydride Transfer in Enzyme Catalysis. Journal of the American Chemical Society, 2000, 122, 8197-8203.	6.6	179
5	Ensemble-averaged variational transition state theory with optimized multidimensional tunneling for enzyme kinetics and other condensed-phase reactions. International Journal of Quantum Chemistry, 2004, 100, 1136-1152.	1.0	122
6	Multi-Coefficient Correlation Method for Quantum Chemistry. Journal of Physical Chemistry A, 1999, 103, 5129-5136.	1.1	110
7	Geometry optimization of molecules in solution: Joint use of the mean field approximation and the free-energy gradient method. Journal of Chemical Physics, 2003, 118, 255-263.	1.2	93
8	ASEP/MD: A program for the calculation of solvent effects combining QM/MM methods and the mean field approximation. Computer Physics Communications, 2003, 155, 244-259.	3.0	85
9	Theoretical Study of the Relative Stability of Rotational Conformers of Î± and Î²-d-Glucopyranose in Gas Phase and Aqueous Solution. Journal of the American Chemical Society, 2004, 126, 7311-7319.	6.6	75
10	The Gaussian-2 method with proper dissociation, improved accuracy, and less cost. Journal of Chemical Physics, 1999, 110, 11679-11681.	1.2	67
11	Quantum mechanical tunneling in methylamine dehydrogenase. Chemical Physics Letters, 2001, 347, 512-518.	1.2	57
12	Theoretical Calculation of the Stark Component of the Soluteâ^'Solvent Interaction Energy. Validity of the Mean Field Approximation in the Study of Liquids and Solutions. Journal of Physical Chemistry B, 2002, 106, 4813-4817.	1.2	52
13	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
14	Importance of Anharmonicity, Recrossing Effects, and Quantum Mechanical Tunneling in Transition State Theory with Semiclassical Tunneling. A Test Case:Â The H2+ Cl Hydrogen Abstraction Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 589-599.	1.1	22
15	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
16	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
17	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
18	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
19	Theoretical study of the role of solvent Stark effect in electron transitions. Theoretical Chemistry Accounts, 2011, 128, 783-793.	0.5	10
20	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
21	Use of the Average Solvent Potential Approach in the Study of Solvent Effects. Advances in Quantum Chemistry, 2010, 59, 59-97.	0.4	2
22	A new QM/MM method oriented to the study of ionic liquids. Journal of Computational Chemistry, 2015, 36, 1893-1901.	1.5	2