Manuel A Aguilar

List of Publications by Year
in descending order

55 papers	1,260 citations	304743 22 h-index	377865 34 g-index
55 all docs	55 docs citations	55 times ranked	1047 citing authors

#	Article	IF	Citations
1	An MP2/Molecular Dynamics study of the solvent effects on the conformational equilibrium of the glycine dipeptide. Journal of Molecular Liquids, 2022, 351, 118557.	4.9	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.	2.5	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.	5.3	8
4	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.	2.8	10
5	Conformational Changes of the Alanine Dipeptide in Waterâ€“Ethanol Binary Mixtures. Journal of Chemical Theory and Computation, 2016, 12, 1514-1524.	5.3	10
6	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.	2.5	13
7	Accelerating QM/MM Calculations by Using the Mean Field Approximation. Challenges and Advances in Computational Chemistry and Physics, 2015, , 135-152.	0.6	0
8	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.	2.5	6
9	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.	2.6	18
10	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.	5.3	12
11	Theoretical Study of the Preferential Solvation Effect on the Solvatochromic Shifts of para-Nitroaniline. Journal of Physical Chemistry B, 2013, 117, 2466-2474.	2.6	24
12	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.	5.3	14
13	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.	1.4	10
14	Dual Fluorescence of Fluorazene in Solution: A Computational Study. Journal of Chemical Theory and Computation, 2011, 7, 3694-3701.	5.3	3
15	Study on the conformational equilibrium of the alanine dipeptide in water solution by using the averaged solvent electrostatic potential from molecular dynamics methodology. Journal of Chemical Physics, 2011, 135, 194502.	3.0	26
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.	5.3	14
17	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.	5.3	26
18	Theoretical study of the role of solvent Stark effect in electron transitions. Theoretical Chemistry Accounts, 2011, 128, 783-793.	1.4	10

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19	On the absorption properties of the excited states of DMABN. Chemical Physics Letters, 2010, 499, 100-102.	2.6	17
20	Use of the Average Solvent Potential Approach in the Study of Solvent Effects. Advances in Quantum Chemistry, 2010, 59, 59-97.	0.8	2
21	Theoretical Study of the Dual Fluorescence of 4-(N,N-Dimethylamino)benzonitrile in Solution. Journal of Chemical Theory and Computation, 2010, 6, 2445-2454.	5.3	35
22	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.	2.6	11
23	Solvatochromic Shifts on Absorption and Fluorescence Bands of N,N-Dimethylaniline. Journal of Chemical Theory and Computation, 2009, 5, 341-349.	5.3	16
24	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.	2.6	12
25	Retinal Models: Comparison of Electronic Absorption Spectra in the Gas Phase and in Methanol Solution. Journal of Physical Chemistry B, 2008, 112, 8815-8823.	2.6	16
26	Solvent Effects on Radiative and Non-Radiative Excited State Decays. Challenges and Advances in Computational Chemistry and Physics, 2008, , 135-157.	0.6	0
27	A CASPT2//CASSCF Study of Vertical and Adiabatic Electron Transitions of Acrolein in Water Solution. Journal of Physical Chemistry B, 2007, 111, 9864-9870.	2.6	34
28	Location of conical intersections in solution using a sequential quantum mechanics/molecular dynamics method. Chemical Physics Letters, 2007, 443, 76-81.	2.6	20
29	Solvent Effects on the Low-Lying Excited States of a Model of Retinal. Journal of Physical Chemistry B, 2006, 110, 18064-18071.	2.6	24
30	An ASEP/MD study of liquid chloroform. Computational and Theoretical Chemistry, 2006, 775, 81-86.	1.5	9
31	Comparison of three effective Hamiltonian models of increasing complexity: Triazene in water as a test case. Journal of Chemical Physics, 2006, 124, 214504.	3.0	10
32	Theoretical Study of the 1,3-Hydrogen Shift of Triazene in Water. Journal of Physical Chemistry B, 2005, 109, 23024-23030.	2.6	16
33	A theoretical study of solvent effects on the 1(nâ†'Ï€*) electron transition in acrolein. Journal of Chemical Physics, 2004, 121, 3710-3716.	3.0	37
34	A new method to locate saddle points for reactions in solution by using the free-energy gradient method and the mean field approximation. Journal of Computational Chemistry, 2004, 25, 1227-1233.	3.3	40
35	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.	13.7	75
36	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.	7.5	85

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37	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
38	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.	3.0	93
39	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.	2.6	52
40	A theoretical study of liquid alcohols using averaged solvent electrostatic potentials obtained from molecular dynamics simulations: Methanol, ethanol and propanol. Journal of Chemical Physics, 2002, 116, 1613-1620.	3.0	47
41	An iterative procedure to determine Lennard-Jones parameters for their use in quantum mechanics/molecular mechanics liquid state simulations. Chemical Physics, 2002, 284, 607-614.	1.9	21
42	Separation of the Electric Polarization into Fast and Slow Components:Â A Comparison of Two Partition Schemes. Journal of Physical Chemistry A, 2001, 105, 10393-10396.	2.5	41
43	A comparative study of two QM/MM methods testing the validity of the mean field approximation. Chemical Physics Letters, 2001, 344, 107-112.	2.6	16
44	Multiconfigurational self-consistent and molecular mechanics simulation of solvent effects on the nâ†'Ï€â^— blue shift of pyrimidine. Computational and Theoretical Chemistry, 2001, 537, 213-222.	1.5	25
45	MÃ¼nchnoneâ^'Alkene Cycloadditions:Â Deviations from the FMO Theory. Theoretical Studies in the Search of the Transition State. Journal of Organic Chemistry, 1996, 61, 7291-7297.	3.2	27
46	Solvent effects on the potential energy surface of the 1:1 complex of water and formamide: Application of the polarizable continuum model to the study of nonadditive effects. Journal of Chemical Physics, 1996, 104, 5539-5546.	3.0	34
47	Nonequilibrium Solvation: The Mutual Influence of Solute and Solvent Dynamics. The Journal of Physical Chemistry, 1995, 99, 4293-4305.	2.9	5
48	Chemical reactions in solution: modelling of the delay of solvent synchronism (dielectric friction) along the reaction path of an SN2 reaction. Chemical Physics, 1993, 174, 397-407.	1.9	24
49	Cavity boundaries in the ab initio polarizable continuum model. Chemical Physics, 1993, 170, 161-165.	1.9	12
50	Correlation and solvation effects. IV. A systematic analysis of the influence of cavity size and shape on solvation properties in the polarizable continuum model with electron correlation. Journal of Computational Chemistry, 1992, 13, 115-134.	3.3	26
51	Electron correlation and solvation effects. II. The description of the vibrational properties of a water molecule in a dielectric given by the application of the polarizable continuum model with inclusion of correlation effects. Chemical Physics, 1991, 150, 151-161.	1.9	54
52	Applications of the basic polarizable continuum model. A study of the vibrational properties of diatomic solutes. Chemical Physics, 1990, 143, 371-379.	1.9	23
53	A computation procedure for the dispersion component of the interaction energy in continuum solute-solvent models. Chemical Physics, 1989, 138, 327-336.	1.9	22
54	Solute-solvent interactions. a simple procedure for constructing the solvent cavity for retaining a molecular solute. Chemical Physics, 1989, 129, 439-450.	1.9	57

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55	Beyond the Continuum Approach. , 0, , 499-605.		6