

# Manuel A Aguilar

## List of Publications by Year in descending order

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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	Geometry optimization of molecules in solution: Joint use of the mean field approximation and the free-energy gradient method. <i>Journal of Chemical Physics</i> , 2003, 118, 255-263.	3.0	93
2	ASEP/MD: A program for the calculation of solvent effects combining QM/MM methods and the mean field approximation. <i>Computer Physics Communications</i> , 2003, 155, 244-259.	7.5	85
3	Theoretical Study of the Relative Stability of Rotational Conformers of $\beta$ - and $\alpha$ -D-Glucopyranose in Gas Phase and Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2004, 126, 7311-7319.	13.7	75
4	Solute-solvent interactions. a simple procedure for constructing the solvent cavity for retaining a molecular solute. <i>Chemical Physics</i> , 1989, 129, 439-450.	1.9	57
5	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. <i>Chemical Physics</i> , 1991, 150, 151-161.	1.9	54
6	Theoretical Calculation of the Stark Component of the Solute-Solvent Interaction Energy. Validity of the Mean Field Approximation in the Study of Liquids and Solutions. <i>Journal of Physical Chemistry B</i> , 2002, 106, 4813-4817.	2.6	52
7	A theoretical study of liquid alcohols using averaged solvent electrostatic potentials obtained from molecular dynamics simulations: Methanol, ethanol and propanol. <i>Journal of Chemical Physics</i> , 2002, 116, 1613-1620.	3.0	47
8	Separation of the Electric Polarization into Fast and Slow Components: A Comparison of Two Partition Schemes. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10393-10396.	2.5	41
9	A new method to locate saddle points for reactions in solution by using the free-energy gradient method and the mean field approximation. <i>Journal of Computational Chemistry</i> , 2004, 25, 1227-1233.	3.3	40
10	A theoretical study of solvent effects on the $n \rightarrow \pi^*$ electron transition in acrolein. <i>Journal of Chemical Physics</i> , 2004, 121, 3710-3716.	3.0	37
11	Theoretical Study of the Dual Fluorescence of 4-(N,N-Dimethylamino)benzonitrile in Solution. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2445-2454.	5.3	35
12	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. <i>Journal of Chemical Physics</i> , 1996, 104, 5539-5546.	3.0	34
13	A CASPT2//CASSCF Study of Vertical and Adiabatic Electron Transitions of Acrolein in Water Solution. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9864-9870.	2.6	34
14	$\pi$ -Alkene Cycloadditions: Deviations from the FMO Theory. <i>Theoretical Studies in the Search of the Transition State</i> . <i>Journal of Organic Chemistry</i> , 1996, 61, 7291-7297.	3.2	27
15	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. <i>Journal of Computational Chemistry</i> , 1992, 13, 115-134.	3.3	26
16	Study on the conformational equilibrium of the alanine dipeptide in water solution by using the averaged solvent electrostatic potential from molecular dynamics methodology. <i>Journal of Chemical Physics</i> , 2011, 135, 194502.	3.0	26
17	Solvent Effects on the Radiative and Nonradiative Decay of a Model of the Rhodopsin Chromophore. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4050-4059.	5.3	26
18	Multiconfigurational self-consistent and molecular mechanics simulation of solvent effects on the $n \rightarrow \pi^*$ blue shift of pyrimidine. <i>Computational and Theoretical Chemistry</i> , 2001, 537, 213-222.	1.5	25

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19	Chemical reactions in solution: modelling of the delay of solvent synchronism (dielectric friction) along the reaction path of an SN2 reaction. <i>Chemical Physics</i> , 1993, 174, 397-407.	1.9	24
20	Solvent Effects on the Low-Lying Excited States of a Model of Retinal. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18064-18071.	2.6	24
21	Theoretical Study of the Preferential Solvation Effect on the Solvatochromic Shifts of <i>p</i> -Nitroaniline. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2466-2474.	2.6	24
22	Applications of the basic polarizable continuum model. A study of the vibrational properties of diatomic solutes. <i>Chemical Physics</i> , 1990, 143, 371-379.	1.9	23
23	A computation procedure for the dispersion component of the interaction energy in continuum solute-solvent models. <i>Chemical Physics</i> , 1989, 138, 327-336.	1.9	22
24	An iterative procedure to determine Lennard-Jones parameters for their use in quantum mechanics/molecular mechanics liquid state simulations. <i>Chemical Physics</i> , 2002, 284, 607-614.	1.9	21
25	Location of conical intersections in solution using a sequential quantum mechanics/molecular dynamics method. <i>Chemical Physics Letters</i> , 2007, 443, 76-81.	2.6	20
26	Theoretical Study of Solvent Effects on the Ground and Low-Lying Excited Free Energy Surfaces of a Push-Pull Substituted Azobenzene. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12518-12530.	2.6	18
27	On the absorption properties of the excited states of DMABN. <i>Chemical Physics Letters</i> , 2010, 499, 100-102.	2.6	17
28	A comparative study of two QM/MM methods testing the validity of the mean field approximation. <i>Chemical Physics Letters</i> , 2001, 344, 107-112.	2.6	16
29	Theoretical Study of the 1,3-Hydrogen Shift of Triazene in Water. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23024-23030.	2.6	16
30	Retinal Models: Comparison of Electronic Absorption Spectra in the Gas Phase and in Methanol Solution. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8815-8823.	2.6	16
31	Solvatochromic Shifts on Absorption and Fluorescence Bands of <i>N,N</i> -Dimethylaniline. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 341-349.	5.3	16
32	Solvent Effects on the Structure and Spectroscopy of the Emitting States of 1-Phenylpyrrole. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1850-1857.	5.3	14
33	Simultaneous Solvent and Counterion Effects on the Absorption Properties of a Model of the Rhodopsin Chromophore. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1548-1556.	5.3	14
34	Substituent and Solvent Effects on the UV-vis Absorption Spectrum of the Photoactive Yellow Protein Chromophore. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5504-5514.	2.5	13
35	Cavity boundaries in the ab initio polarizable continuum model. <i>Chemical Physics</i> , 1993, 170, 161-165.	1.9	12
36	Solvent Effects on Internal Conversions and Intersystem Crossings: The Radiationless De-Excitation of Acrolein in Water. <i>Journal of Physical Chemistry B</i> , 2008, 112, 877-884.	2.6	12

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37	Solvent Effects on the Absorption Spectra of the <i>para</i> -Coumaric Acid Chromophore in Its Different Protonation Forms. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4481-4494.	5.3	12
38	Theoretical Study of the Competition between Intramolecular Hydrogen Bonds and Solvation in the Cys-Asn-Ser Tripeptide. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8961-8970.	2.6	11
39	Comparison of three effective Hamiltonian models of increasing complexity: Triazene in water as a test case. <i>Journal of Chemical Physics</i> , 2006, 124, 214504.	3.0	10
40	Theoretical study of the role of solvent Stark effect in electron transitions. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 783-793.	1.4	10
41	Theoretical study of the conformational equilibrium of 1,4-dioxane in gas phase, neat liquid, and dilute aqueous solutions. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	1.4	10
42	Solvent effects on de-excitation channels in the <i>p</i> -coumaric acid methyl ester anion, an analogue of the photoactive yellow protein (PYP) chromophore. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27476-27485.	2.8	10
43	Conformational Changes of the Alanine Dipeptide in Water-Ethanol Binary Mixtures. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1514-1524.	5.3	10
44	An ASEP/MD study of liquid chloroform. <i>Computational and Theoretical Chemistry</i> , 2006, 775, 81-86.	1.5	9
45	QM/MM Study of Substituent and Solvent Effects on the Excited State Dynamics of the Photoactive Yellow Protein Chromophore. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 737-748.	5.3	8
46	Beyond the Continuum Approach. , 0, , 499-605.		6
47	Theoretical study of the absorption and emission spectra of the anionic <i>p</i> -coumaric methyl ester in gas phase and in solution. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 287-294.	2.5	6
48	How Methylation Modifies the Photophysics of the Native All- <i>trans</i> -Retinal Protonated Schiff Base: A CASPT2/MD Study in Gas Phase and in Methanol. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3096-3106.	2.5	6
49	Nonequilibrium Solvation: The Mutual Influence of Solute and Solvent Dynamics. <i>The Journal of Physical Chemistry</i> , 1995, 99, 4293-4305.	2.9	5
50	An averaged solvent electrostatic potential/molecular dynamics study of the influence of the electron correlation on the properties of liquid hydrogen fluoride. <i>Computational and Theoretical Chemistry</i> , 2003, 632, 227-234.	1.5	3
51	Dual Fluorescence of Fluorazene in Solution: A Computational Study. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3694-3701.	5.3	3
52	An MP2/Molecular Dynamics study of the solvent effects on the conformational equilibrium of the glycine dipeptide. <i>Journal of Molecular Liquids</i> , 2022, 351, 118557.	4.9	3
53	Use of the Average Solvent Potential Approach in the Study of Solvent Effects. <i>Advances in Quantum Chemistry</i> , 2010, 59, 59-97.	0.8	2
54	Solvent Effects on Radiative and Non-Radiative Excited State Decays. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008, , 135-157.	0.6	0

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55	Accelerating QM/MM Calculations by Using the Mean Field Approximation. Challenges and Advances in Computational Chemistry and Physics, 2015, , 135-152.	0.6	0