

# Antonio Hidalgo

## List of Publications by Year in descending order

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57  
papers

617  
citations

706676

14  
h-index

799663

21  
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58  
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58  
docs citations

58  
times ranked

596  
citing authors

#	ARTICLE	IF	CITATIONS
1	Experimental Design and Optimization of a Novel Dual-release Drug Delivery System With Therapeutic Potential Against Infection With <i>Helicobacter pylori</i> . <i>Colloids and Surfaces B: Biointerfaces</i> , 2022, 213, 112403.	2.5	2
2	[Translated article] Spanish Asthma Management Guidelines (GEMA) v.5.1. Highlights and Controversies. <i>Archivos De Bronconeumologia</i> , 2022, 58, T150-T158.	0.4	7
3	Mechanisms of the T-A to C-G transition studied by SMD simulations: Deamination vs tautomerisation. <i>Journal of Molecular Liquids</i> , 2020, 308, 113036.	2.3	6
4	A procedure to understanding the C-G to A-T transversion. SMD simulations from guanine oxidation pathways assisted by one H <sub>2</sub> O <sub>2</sub> molecule in the C-G basis pair. <i>Journal of Molecular Liquids</i> , 2020, 319, 114123.	2.3	0
5	Theoretical Study of Adenine to Guanine Transition Assisted by Water and Formic Acid Using Steered Molecular Dynamic Simulations. <i>Frontiers in Chemistry</i> , 2019, 7, 414.	1.8	9
6	Photocatalysis in an external four-lamp reactor: modelling and validation of dichloroacetic acid photo-oxidation in the presence of TiO <sub>2</sub> . <i>International Journal of Environmental Science and Technology</i> , 2019, 16, 6705-6716.	1.8	5
7	Structural and thermodynamic studies of cytosine to thymine conversion in gas and solution phases using steered molecular dynamic simulations. <i>Journal of Molecular Liquids</i> , 2019, 278, 61-69.	2.3	9
8	Mechanisms for guanine-cytosine tautomeric equilibrium in solution via steered molecular dynamic simulations. <i>Journal of Molecular Liquids</i> , 2018, 251, 308-316.	2.3	18
9	Neuroprotective effect of a new variant of Epo nonhematopoietic against oxidative stress. <i>Redox Biology</i> , 2018, 14, 285-294.	3.9	23
10	Theoretical study of mechanisms for the hydrolytic deamination of cytosine via steered molecular dynamic simulations. <i>RSC Advances</i> , 2018, 8, 34867-34876.	1.7	5
11	Theoretical study of mechanisms for double proton transfer in adenine-uracil base pair via steered molecular dynamic simulations. <i>Journal of Molecular Liquids</i> , 2018, 265, 487-495.	2.3	4
12	Steered molecular dynamic simulations of the tautomeric equilibria in solution of DNA bases. <i>Journal of Molecular Liquids</i> , 2017, 237, 81-88.	2.3	16
13	A New Malleostapedotomy Prosthesis. Experimental Analysis by Laser Doppler Vibrometer in Fresh Cadaver Temporal Bones. <i>Acta Otorrinolaringologica (English Edition)</i> , 2017, 68, 69-79.	0.1	0
14	Theoretical thermodynamic study of the adenine-thymine tautomeric equilibrium: Electronic structure calculations and steered molecular dynamic simulations. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25429.	1.0	17
15	Theoretical determination of aqueous acid-base pK values: electronic structure calculations and steered molecular dynamic simulations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	9
16	Theoretical study of enzymatically catalyzed tautomerization of carbon acids in aqueous solution: quantum calculations and steered molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , 2016, 22, 44.	0.8	3
17	A computational model of the glycine tautomerization reaction in aqueous solution. <i>Journal of Molecular Modeling</i> , 2014, 20, 2147.	0.8	4
18	Amide-imide tautomerism of acetohydroxamic acid in aqueous solution: quantum calculation and SMD simulations. <i>RSC Advances</i> , 2014, 4, 44757-44768.	1.7	21

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19	Thermodynamic Study of Hydrolysis Reactions in Aqueous Solution from Ab Initio Potential and Molecular Dynamics Simulations. <i>Journal of Chemistry</i> , 2013, 2013, 1-8.	0.9	1
20	Amino Acid Tautomerization Reactions in Aqueous Solution via Concerted and Assisted Mechanisms Using Free Energy Curves from MD Simulation. <i>Journal of Physical Chemistry B</i> , 2012, 116, 13033-13044.	1.2	11
21	Theoretical study of the neutral hydrolysis of methyl formate via a concerted and stepwise water-assisted mechanism using free-energy curves and molecular dynamics simulation. <i>Structural Chemistry</i> , 2011, 22, 909-915.	1.0	9
22	Molecular dynamics study of formamidine decomposition in gas and solution phases via free energy curves from ab initio interaction potentials. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 671-679.	0.5	7
23	Is the middle ear the first filter of frequency selectivity?. <i>Acta Otorrinolaringologica (English)</i> Tj ETQq1 1 0.784314 rgBT /Overlock 10 10 0.1	0.1	3
24	Theoretical Study of the Neutral Hydrolysis of Hydrogen Isocyanate in Aqueous Solution via Assisted-Concerted Mechanisms. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1858-1863.	1.1	15
25	Calculation of free-energy curves for the study of hydrolysis reactions in aqueous solution from ab initio potentials and molecular dynamics simulation. <i>Chemical Physics</i> , 2008, 353, 73-78.	0.9	14
26	Molecular Simulation of the Hydration of Ethene to Ethanol Using Ab Initio Potentials and Free Energy Curves. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13515-13520.	1.1	10
27	Molecular Dynamics Simulation of the Reaction of Hydration of Formaldehyde Using a Potential Based on Solute-Solvent Interaction Energy Components. <i>Journal of Physical Chemistry A</i> , 2007, 111, 339-344.	1.1	20
28	Molecular dynamics simulation of acetamide solvation using interaction energy components: Application to structural and energy properties. <i>Chemical Physics</i> , 2006, 327, 187-192.	0.9	13
29	Theoretical-experimental study of the solvation enthalpy of acetone in dilute aqueous solution. <i>Chemical Physics</i> , 2005, 315, 76-80.	0.9	12
30	Molecular Dynamics Simulation of Aqueous Solutions Using Interaction Energy Components: Application to the Solvation Gibbs Energy. <i>Journal of Solution Chemistry</i> , 2005, 34, 407-414.	0.6	12
31	Molecular dynamics simulation of aqueous solutions using interaction energy components: Application to the dielectric properties of the acetone-water system. <i>Molecular Simulation</i> , 2005, 31, 549-553.	0.9	5
32	Accuracy of high-resolution CT in distinguishing between <i>Pneumocystis carinii</i> pneumonia and non- <i>Pneumocystis carinii</i> pneumonia in AIDS patients. <i>European Radiology</i> , 2003, 13, 1179-1184.	2.3	94
33	Thermodynamic and dielectric properties of aqueous solutions using ESIE charges to describe small solutes. <i>Chemical Physics</i> , 2003, 293, 193-202.	0.9	11
34	Relation between alcohol consumption and the success of <i>Helicobacter pylori</i> eradication therapy using omeprazole, clarithromycin and amoxicillin for 1 week. <i>European Journal of Gastroenterology and Hepatology</i> , 2002, 14, 291-296.	0.8	36
35	The N-H <sup>+</sup> O <sup>-</sup> ...C proton transfer in aqueous solution: a suitable procedure for extracting atomic charges. <i>Chemical Physics Letters</i> , 2002, 357, 279-286.	1.2	15
36	Study of the N-H <sup>+</sup> O <sup>-</sup> ...C proton transfer reaction in aqueous solution using classical free energy curves. <i>Chemical Physics</i> , 2001, 265, 207-215.	0.9	4

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37	Thermodynamic, structural, and dynamic study of the Nâ€“Hâ€“O...C hydrogen bond association in aqueous solution. <i>Chemical Physics</i> , 2000, 255, 73-84.	0.9	12
38	Title is missing!. <i>Journal of Solution Chemistry</i> , 1999, 28, 1087-1106.	0.6	6
39	Quiz case I. <i>European Journal of Radiology</i> , 1998, 27, 250-253.	1.2	6
40	Nonequilibrium Solvation: The Mutual Influence of Solute and Solvent Dynamics. <i>The Journal of Physical Chemistry</i> , 1995, 99, 4293-4305.	2.9	5
41	Self-consistent-field calculation of vibrational bound states for triatomic molecules using transformed Jacobi coordinates. <i>The Journal of Physical Chemistry</i> , 1991, 95, 2292-2297.	2.9	17
42	Variational calculation of vibrational energies of triatomic molecules using SCFOptimized modes. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 685-694.	1.0	14
43	Energy eigenvalues for Lennard-Jones potentials using the hypervirial perturbative method. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 1990, 23, 2771-2781.	0.6	11
44	Twoâ€“center matrix elements for Kratzer oscillators. <i>Journal of Chemical Physics</i> , 1990, 93, 3408-3412.	1.2	15
45	Perturbative virtual SCF Ctreatment for energy levels of coupled oscillator systems. <i>International Journal of Quantum Chemistry</i> , 1989, 36, 49-60.	1.0	2
46	SCF calculations of excited vibrational energy levels for normal modes. <i>Computational and Theoretical Chemistry</i> , 1988, 166, 339-344.	1.5	0
47	Perturbative multi-step adiabatic treatment for energy levels of multidimensional coupled systems. <i>Computational and Theoretical Chemistry</i> , 1988, 166, 345-350.	1.5	0
48	Variational HEG calculation of vibration rotation transition moments for diatomic molecules.. <i>Computational and Theoretical Chemistry</i> , 1988, 166, 351-356.	1.5	0
49	Perturbed Morse expansion for triatomic molecules. <i>Computational and Theoretical Chemistry</i> , 1988, 166, 357-362.	1.5	1
50	Analytical expressions for vibrational matrix elements of Morse oscillators. <i>Physical Review A</i> , 1988, 38, 4205-4212.	1.0	9
51	Perturbative calculation of energy levels for coupled oscillators using the adiabatic approximation. <i>Molecular Physics</i> , 1987, 61, 1513-1518.	0.8	1
52	Hypervirial SCF treatment for vibrational energy levels of triatomic molecules. <i>International Journal of Quantum Chemistry</i> , 1987, 32, 511-516.	1.0	2
53	Perturbative calculation of vibrational energy levels for local modes. <i>Journal De Chimie Physique Et De Physico-Chimie Biologique</i> , 1987, 84, 725-728.	0.2	0
54	Rovibrational energy levels and expectation values for perturbed Kratzer oscillators. <i>Journal of Chemical Physics</i> , 1986, 85, 3939-3944.	1.2	18

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55	Determination of the degree of branching in polyethylene by an i.r. method of decomposition of bands. Spectrochimica Acta Part A: Molecular Spectroscopy, 1979, 35, 847-849.	0.1	21
56	An i.r. study of the "amorphous" phase in melt crystallized polyethylene. Spectrochimica Acta Part A: Molecular Spectroscopy, 1978, 34, 475-480.	0.1	14
57	Correlation of crystal thickness and absorption coefficient of the doublet at 720-730 cm <sup>-1</sup> in polyethylene. Journal of Polymer Science, Polymer Physics Edition, 1977, 15, 2027-2031.	1.0	11