Guillermo Prez-Hernndez

List of Publications by Year in Descending Order

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Version: 2024-04-27

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

16 papers	1,474 citations	12 h-index	17 g-index
17 ext. papers	1,891 ext. citations	3.9 avg, IF	4.49 L-index

#	Paper	IF	Citations
16	Defining the architecture of KPC-2 Carbapenemase: identifying allosteric networks to fight antibiotics resistance. *Scientific Reports*, **2018**, 8, 12916	4.9	19
15	Exploring the Dynamics of Propeller Loops in Human Telomeric DNA Quadruplexes Using Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 2458-2480	6.4	30
14	Hierarchical Time-Lagged Independent Component Analysis: Computing Slow Modes and Reaction Coordinates for Large Molecular Systems. *Journal of Chemical Theory and Computation*, **2016**, 12, 6118-6129	6.4	41
13	PyEMMA 2: A Software Package for Estimation, Validation, and Analysis of Markov Models. *Journal of Chemical Theory and Computation*, **2015**, 11, 5525-42	6.4	504
12	Variational Approach to Molecular Kinetics. *Journal of Chemical Theory and Computation*, **2014**, 10, 1739-52	6.4	193
11	Anisotropy of the water-carbon interaction: molecular simulations of water in low-diameter carbon nanotubes. *Physical Chemistry Chemical Physics*, **2013**, 15, 4995-5006	3.6	26
10	Identification of slow molecular order parameters for Markov model construction. *Journal of Chemical Physics*, **2013**, 139, 015102	3.9	522
9	IR spectrum of FHF- and FDF- revisited using a spectral method in four dimensions. *Journal of Physical Chemistry A*, **2012**, 116, 11361-9	2.8	16
8	Singlet oxygen generation versus O–O homolysis in phenyl-substituted anthracene endoperoxides investigated by RASPT2, CASPT2, CC2, and TD-DFT methods. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	5
7	On the light-driven isomerization of a model asymmetric molecular rotor: conformations and conical intersections of 2-cyclopentylidene-tetrahydrofuran. *Journal of Physical Chemistry A*, **2010**, 114, 9342-8	2.8	12
6	Mechanistic insight into light-driven molecular rotors: a conformational search in chiral overcrowded alkenes by a pseudo-random approach. *Physical Chemistry Chemical Physics*, **2010**, 12, 12279-89	3.6	20
5	Biologically inspired molecular machines driven by light. Optimal control of a unidirectional rotor. *New Journal of Physics*, **2010**, 12, 075007	2.9	22
4	Excited state dynamics of a model asymmetric molecular rotor: A five-dimensional study on 2-cyclopentylidene-tetrahydrofuran. *Chemical Physics*, **2010**, 377, 86-95	2.3	10
3	The chromophore structure of the cyanobacterial phytochrome Cph1 as predicted by time-dependent density functional theory. *Journal of Physical Chemistry B*, **2008**, 112, 16253-6	3.4	32
2	Towards Toroidal Hydrogen Bonds. *Zeitschrift Fur Physikalische Chemie*, **2008**, 222, 1311-1331	3.1	12
1	Rydberg or valence? The long-standing question in the UV absorption spectrum of 1,1′-bicyclohexylidene. *ChemPhysChem*, **2008**, 9, 2544-9	3.2	10