

Guillermo PÃ©rez-HernÃ¡ndez

List of Publications by Year in descending order

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16
papers

2,217
citations

759233

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940533

16
g-index

17
all docs

17
docs citations

17
times ranked

2013
citing authors

#	ARTICLE	IF	CITATIONS
1	Defining the architecture of KPC-2 Carbapenemase: Identifying allosteric networks to fight antibiotics resistance. Scientific Reports, 2018, 8, 12916.	3.3	27
2	Exploring the Dynamics of Propeller Loops in Human Telomeric DNA Quadruplexes Using Atomistic Simulations. Journal of Chemical Theory and Computation, 2017, 13, 2458-2480.	5.3	39
3	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.	5.3	57
4	PyEMMA 2: A Software Package for Estimation, Validation, and Analysis of Markov Models. Journal of Chemical Theory and Computation, 2015, 11, 5525-5542.	5.3	876
5	Variational Approach to Molecular Kinetics. Journal of Chemical Theory and Computation, 2014, 10, 1739-1752.	5.3	256
6	Anisotropy of the water-carbon interaction: molecular simulations of water in low-diameter carbon nanotubes. Physical Chemistry Chemical Physics, 2013, 15, 4995.	2.8	36
7	Identification of slow molecular order parameters for Markov model construction. Journal of Chemical Physics, 2013, 139, 015102.	3.0	777
8	IR Spectrum of FHF ⁺ and FDF ⁺ Revisited Using a Spectral Method in Four Dimensions. Journal of Physical Chemistry A, 2012, 116, 11361-11369.	2.5	16
9	Singlet oxygen generation versus O ⁺ homolysis in phenyl-substituted anthracene endoperoxides investigated by RASPT2, CASPT2, CC2, and TD-DFT methods. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	5
10	Biologically inspired molecular machines driven by light. Optimal control of a unidirectional rotor. New Journal of Physics, 2010, 12, 075007.	2.9	22
11	Excited state dynamics of a model asymmetric molecular rotor: A five-dimensional study on 2-cyclopentylidene-tetrahydrofuran. Chemical Physics, 2010, 377, 86-95.	1.9	10
12	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, 9342-9348.	2.5	12
13	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.	2.8	21
14	Rydberg or Valence? The Long-standing Question in the UV Absorption Spectrum of 1,1a ² -Bicyclohexylidene. ChemPhysChem, 2008, 9, 2544-2549.	2.1	11
15	The Chromophore Structure of the Cyanobacterial Phytochrome Cph1 As Predicted by Time-Dependent Density Functional Theory. Journal of Physical Chemistry B, 2008, 112, 16253-16256.	2.6	33
16	Towards Toroidal Hydrogen Bonds. Zeitschrift Fur Physikalische Chemie, 2008, 222, 1311-1331.	2.8	14