

Guillermo Prez-Hernandez

List of Publications by Citations

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