Jose M Borreguero

List of Publications by Year
in descending order

28 papers	2,511 citations	516710 16 h-index	580821 25 g-index
29 all docs	29 docs citations	29 times ranked	4171 citing authors

#	Article	IF	Citations
1	Modulating Enzyme Activity by Altering Protein Dynamics with Solvent. Biochemistry, 2018, 57, 4263-4275.	2.5	26
2	idpflex: Analysis of Intrinsically Disordered Proteins by Comparing Simulations to Small Angle Scattering Experiments. Journal of Open Source Software, 2018, 3, 1007.	4.6	2
3	Unraveling the Agglomeration Mechanism in Charged Block Copolymer and Surfactant Complexes. Macromolecules, 2017, 50, 1193-1205.	4.8	30
4	Disruption of Hydrogen-Bonding Network Eliminates Water Anomalies Normally Observed on Cooling to Its Calorimetric Glass Transition. Journal of Physical Chemistry B, 2017, 121, 4168-4173.	2.6	3
5	Dynamics of Charged Species in Ionic-Neutral Block Copolymer and Surfactant Complexes. Journal of Physical Chemistry B, 2017, 121, 6958-6968.	2.6	9
6	An automated analysis workflow for optimization of force-field parameters using neutron scattering data. Journal of Computational Physics, 2017, 340, 128-137.	3.8	10
7	BEAM: A Computational Workflow System for Managing and Modeling Material Characterization Data in HPC Environments. Procedia Computer Science, 2016, 80, 2276-2280.	2.0	17
8	Precise determination of water exchanges on a mineral surface. Physical Chemistry Chemical Physics, 2016, 18, 28819-28828.	2.8	20
9	Molecular Dynamics Force-Field Refinement against Quasi-Elastic Neutron Scattering Data. Journal of Chemical Theory and Computation, 2016, 12, 9-17.	5.3	9
10	Self-assembly and structural relaxation in a model ionomer melt. Journal of Chemical Physics, 2015, 142, 084903.	3.0	6
11	Surfactant-Mediated Polyelectrolyte Self-Assembly in a Polyelectrolyteâ€“Surfactant Complex. Macromolecules, 2015, 48, 9050-9059.	4.8	49
12	Mantidâ€”Data analysis and visualization package for neutron scattering and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0002.gif" overflow="scroll"><mml:mi mathvariant="normal">Î¼</mml:mi></mml:math> SR experiments. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2014, 764, 156-166.	1.6	1,257
13	Integrating Advanced Materials Simulation Techniques into an Automated Data Analysis Workflow at the Spallation Neutron Source. , 2014, , 297-308.		1
14	Learning Protein Folding Energy Functions. , 2011, , 1062-1067.		4
15	Redox-Promoting Protein Motions in Rubredoxin. Journal of Physical Chemistry B, 2011, 115, 8925-8936.	2.6	14
16	Protein Flexibility and Energy Flow During Enzyme Catalysis. Biophysical Journal, 2011, 100, 194a.	0.5	0
17	Parallel Folding Pathways in the SH3 Domain Protein. Journal of Molecular Biology, 2007, 373, 1348-1360.	4.2	29
18	Benchmarking of TASSER in the ab initio limit. Proteins: Structure, Function and Bioinformatics, 2007, 68, 48-56.	2.6	9

#	Article	IF	Citations
19	Analysis of TASSER-based CASP7 protein structure prediction results. Proteins: Structure, Function and Bioinformatics, 2007, 69, 90-97.	2.6	61
20	Elucidating Amyloid Î²-Protein Folding and Assembly:â€‰ A Multidisciplinary Approach. Accounts of Chemical Research, 2006, 39, 635-645.	15.6	203
21	Ab initio Discrete Molecular Dynamics Approach to Protein Folding and Aggregation. Methods in Enzymology, 2006, 412, 314-338.	1.0	65
22	Folding events in the 21-30 region of amyloid Â-protein (AÂ) studied in silico. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6015-6020.	7.1	122
23	Solvent and mutation effects on the nucleation of amyloid Â-protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 18258-18263.	7.1	113
24	Multiple Folding Pathways of the SH3 Domain. Biophysical Journal, 2004, 87, 521-533.	0.5	38
25	Possible Mechanism for Cold Denaturation of Proteins at High Pressure. Physical Review Letters, 2003, 91, 138103.	7.8	95
26	Mechanism for the ?-helix to ?-hairpin transition. Proteins: Structure, Function and Bioinformatics, 2003, 53, 220-228.	2.6	252
27	Identifying Importance of Amino Acids for Protein Folding from Crystal Structures. Methods in Enzymology, 2003, 374, 616-638.	1.0	12
28	Thermodynamics and Folding Kinetics Analysis of the SH3 Domain form Discrete Molecular Dynamics. Journal of Molecular Biology, 2002, 318, 863-876.	4.2	54