Patrick Senet

List of Publications by Year
in descending order

35 papers	832 citations	471509 17 h-index	477307 29 g-index
37 all docs	37 docs citations	37 times ranked	1095 citing authors

#	Article	IF	Citations
1	Angstrom-Size Defect Creation and Ionic Transport through Pores in Single-Layer MoS₂. Nano Letters, 2018, 18, 1651-1659.	9.1	129
2	Investigation of Protein Folding by Coarse-Grained Molecular Dynamics with the UNRES Force Field. Journal of Physical Chemistry A, 2010, 114, 4471-4485.	2.5	91
3	DFT study of polarizabilities and dipole moments of water clusters. International Journal of Quantum Chemistry, 2005, 101, 535-542.	2.0	70
4	Simulation of the Opening and Closing of Hsp70 Chaperones by Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 1750-1764.	5.3	63
5	How main-chains of proteins explore the free-energy landscape in native states. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 19708-19713.	7.1	52
6	Decipher the Mechanisms of Protein Conformational Changes Induced by Nucleotide Binding through Free-Energy Landscape Analysis: ATP Binding to Hsp70. PLoS Computational Biology, 2013, 9, e1003379.	3.2	30
7	Anomalous diffusion and dynamical correlation between the side chains and the main chain of proteins in their native state. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 10346-10351.	7.1	29
8	Influence of Structure on the Polarizability of Hydrated Methane Sulfonic Acid Clusters. Journal of Chemical Theory and Computation, 2008, 4, 2122-2129.	5.3	28
9	Local softness, softness dipole, and polarizabilities of functional groups: Application to the side chains of the 20 amino acids. Journal of Chemical Physics, 2009, 131, 044312.	3.0	28
10	Nonexponential decay of internal rotational correlation functions of native proteins and self-similar structural fluctuations. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 19844-19849.	7.1	28
11	Reconstructing the free-energy landscape of Met-enkephalin using dihedral principal component analysis and well-tempered metadynamics. Journal of Chemical Physics, 2013, 138, 235101.	3.0	26
12	Human Inducible Hsp70: Structures, Dynamics, and Interdomain Communication from All-Atom Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2010, 6, 2501-2519.	5.3	25
13	Effect of Structural Parameters on the Polarizabilities of Methanol Clusters:â€‰ A Hirshfeld Study. Journal of Chemical Theory and Computation, 2008, 4, 426-434.	5.3	24
14	From a Highly Disordered to a Metastable State: Uncovering Insights of Î±-Synuclein. ACS Chemical Neuroscience, 2018, 9, 1051-1065.	3.5	22
15	New Insights into Protein (Un)Folding Dynamics. Journal of Physical Chemistry Letters, 2015, 6, 1082-1086.	4.6	20
16	Improved model of ionic transport in 2-D MoS2 membranes with sub-5â€‰nm pores. Applied Physics Letters, 2019, 114, 023107.	3.3	19
17	Local vs Global Motions in Protein Folding. Journal of Chemical Theory and Computation, 2013, 9, 2907-2921.	5.3	18
18	Conformational dynamics of full-length inducible human Hsp70 derived from microsecond molecular dynamics simulations in explicit solvent. Journal of Biomolecular Structure and Dynamics, 2013, 31, 1111-1126.	3.5	16

#	Article	IF	Citations
19	Molecular Dynamics Investigation of Polylysine Peptide Translocation through MoS₂ Nanopores. Journal of Physical Chemistry B, 2019, 123, 2342-2353.	2.6	15
20	Intrinsic Localized Modes in Proteins. Scientific Reports, 2015, 5, 18128.	3.3	11
21	Fingerprints of Conformational States of Human Hsp70 at Sub-THz Frequencies. ACS Omega, 2016, 1, 1067-1074.	3.5	11
22	Investigation of Phosphorylation-Induced Folding of an Intrinsically Disordered Protein by Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 3203-3220.	5.3	11
23	Theoretical Insights into Sub-Terahertz Acoustic Vibrations of Proteins Measured in Single-Molecule Experiments. Journal of Physical Chemistry Letters, 2016, 7, 5128-5136.	4.6	10
24	Curvature and Torsion of Protein Main Chain as Local Order Parameters of Protein Unfolding. Journal of Physical Chemistry B, 2020, 124, 4391-4398.	2.6	9
25	Missense Mutations Modify the Conformational Ensemble of the Î±-Synuclein Monomer Which Exhibits a Two-Phase Characteristic. Frontiers in Molecular Biosciences, 2021, 8, 786123.	3.5	9
26	Nanopore sensing of single-biomolecules: a new procedure to identify protein sequence motifs from molecular dynamics. Nanoscale, 2020, 12, 22743-22753.	5.6	8
27	Wild-Type Î±-Synuclein and Variants Occur in Different Disordered Dimers and Pre-Fibrillar Conformations in Early Stage of Aggregation. Frontiers in Molecular Biosciences, 0, 9, .	3.5	7
28	Low-Frequency, Functional, Modes of Proteins: All-Atom and Coarse-Grained Normal Mode Analysis. Springer Series in Bio-/neuroinformatics, 2014, , 483-524.	0.1	6
29	Statistical Model To Decipher Protein Folding/Unfolding at a Local Scale. Journal of Physical Chemistry B, 2018, 122, 3540-3549.	2.6	6
30	New Insights into Folding, Misfolding, and Nonfolding Dynamics of a WW Domain. Journal of Physical Chemistry B, 2020, 124, 3855-3872.	2.6	4
31	Variational Principle for Eigenmodes of Reactivity in Conceptual Density Functional Theory. ACS Omega, 2020, 5, 25349-25357.	3.5	3
32	Challenges in Protein Sequencing Using 2-D MoS$$_2$$ Nanopores. Nanostructure Science and Technology, 2022, , 343-366.	0.1	1
33	An ab initio softness metric to measure the similarity between all pairs of amino acids. Computational and Theoretical Chemistry, 2010, 943, 103-109.	1.5	0
34	Deciphering Molecular Complexity in Dynamics and Kineticsâ€"From the Single Molecule to the Single Cell Level. Journal of Physical Chemistry B, 2019, 123, 6387-6388.	2.6	0
35	Raman and Infrared Spectra of Acoustical, Functional Modes of Proteins from All-Atom and Coarse-Grained Normal Mode Analysis. Springer Series on Bio- and Neurosystems, 2019, , 501-539.	0.2	0