Mahmoud Moradi

List of Publications by Year
in descending order

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49	1,003	516710 16	477307 29
papers	citations	h-index	g-index

63	63	63	1090
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mechanistic picture for conformational transition of a membrane transporter at atomic resolution. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 18916-18921.	7.1	140
2	Atomic-level characterization of transport cycle thermodynamics in the glycerol-3-phosphate:phosphate antiporter. Nature Communications, 2015, 6, 8393.	12.8	97
3	Conformations and free energy landscapes of polyproline peptides. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 20746-20751.	7.1	92
4	Computational Recipe for Efficient Description of Large-Scale Conformational Changes in Biomolecular Systems. Journal of Chemical Theory and Computation, 2014, 10, 2866-2880.	5.3	73
5	Computational characterization of structural dynamics underlying function in active membrane transporters. Current Opinion in Structural Biology, 2015, 31, 96-105.	5.7	49
6	Reaction path ensemble of the Bâ€“Z-DNA transition: a comprehensive atomistic study. Nucleic Acids Research, 2013, 41, 33-43.	14.5	48
7	Chemomechanical Coupling in Hexameric Proteinâ€“Protein Interfaces Harnesses Energy within V-Type ATPases. Journal of the American Chemical Society, 2017, 139, 293-310.	13.7	44
8	Adaptively biased molecular dynamics: An umbrella sampling method with a timeâ€dependent potential. International Journal of Quantum Chemistry, 2009, 109, 3666-3678.	2.0	35
9	Lipid-Dependent Alternating Access Mechanism of a Bacterial Multidrug ABC Exporter. ACS Central Science, 2019, 5, 43-56.	11.3	35
10	A classical molecular dynamics investigation of the free energy and structure of short polyproline conformers. Journal of Chemical Physics, 2010, 133, 125104.	3.0	32
11	Driven Metadynamics: Reconstructing Equilibrium Free Energies from Driven Adaptive-Bias Simulations. Journal of Physical Chemistry Letters, 2013, 4, 1882-1887.	4.6	29
12	What Can and Cannot Be Learned from Molecular Dynamics Simulations of Bacterial Proton-Coupled Oligopeptide Transporter GkPOT?. Journal of Physical Chemistry B, 2017, 121, 3644-3656.	2.6	27
13	A Statistical Analysis of the PPII Propensity of Amino Acid Guests in Proline-Rich Peptides. Biophysical Journal, 2011, 100, 1083-1093.	0.5	24
14	ALS-causing mutations in profilin-1 alter its conformational dynamics: A computational approach to explain propensity for aggregation. Scientific Reports, 2018, 8, 13102.	3.3	19
15	Calculating relative transition rates with driven nonequilibrium simulations. Chemical Physics Letters, 2011, 518, 109-113.	2.6	18
16	Are Long-Range Structural Correlations Behind the Aggregration Phenomena of Polyglutamine Diseases?. PLoS Computational Biology, 2012, 8, e1002501.	3.2	18
17	PPII Propensity of Multiple-Guest Amino Acids in a Proline-Rich Environment. Journal of Physical Chemistry B, 2011, 115, 8645-8656.	2.6	17
18	Characterizing a Histidine Switch Controlling pH-Dependent Conformational Changes of the Influenza Virus Hemagglutinin. Biophysical Journal, 2013, 105, 993-1003.	0.5	17

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19	Prefusion spike protein conformational changes are slower in SARS-CoV-2 than in SARS-CoV-1. Journal of Biological Chemistry, 2022, 298, 101814.	3.4	17
20	Free energy and structure of polyproline peptides: An ab initio and classical molecular dynamics investigation. International Journal of Quantum Chemistry, 2010, 110, 2865-2879.	2.0	16
21	Conformational Dynamics at the Inner Gate of KcsA during Activation. Biochemistry, 2014, 53, 2557-2559.	2.5	16
22	Investigating rare events with nonequilibrium work measurements. I. Nonequilibrium transition path probabilities. Journal of Chemical Physics, 2014, 140, 034114.	3.0	14
23	A Companion Guide to the String Method with Swarms of Trajectories: Characterization, Performance, and Pitfalls. Journal of Chemical Theory and Computation, 2022, 18, 1406-1422.	5.3	14
24	Investigating rare events with nonequilibrium work measurements. II. Transition and reaction rates. Journal of Chemical Physics, 2014, 140, 034115.	3.0	13
25	High school biology students use of visual molecular dynamics as an authentic tool for learning about modeling as a professional scientific practice. Biochemistry and Molecular Biology Education, 2018, 46, 230-236.	1.2	13
26	The Adaptively Biased Molecular Dynamics method revisited: New capabilities and an application. Journal of Physics: Conference Series, 2015, 640, 012020.	0.4	12
27	Effective Riemannian Diffusion Model for Conformational Dynamics of Biomolecular Systems. Journal of Physical Chemistry Letters, 2016, 7, 4980-4987.	4.6	12
28	The Role of a Crystallographically Unresolved Cytoplasmic Loop in Stabilizing the Bacterial Membrane Insertase YidC2. Scientific Reports, 2019, 9, 14451.	3.3	9
29	Recipes for Free Energy Calculations in Biomolecular Systems. Methods in Molecular Biology, 2013, 924, 313-337.	0.9	6
30	Characterization of the structural forces governing the reversibility of the thermal unfolding of the human acidic fibroblast growth factor. Scientific Reports, 2021, 11, 15579.	3.3	5
31	Elucidating the molecular basis of spontaneous activation in an engineered mechanosensitive channel. Computational and Structural Biotechnology Journal, 2022, 20, 2539-2550.	4.1	5
32	A Microscopic View of the Mechanisms of Active Transport Across the Cellular Membrane. Annual Reports in Computational Chemistry, 2014, 10, 77-125.	1.7	4
33	Molecular Dynamicsâ€“Based Thermodynamic and Kinetic Characterization of Membrane Protein Conformational Transitions. Methods in Molecular Biology, 2021, 2302, 289-309.	0.9	4
34	Mechanistic Picture for Monomeric Human Fibroblast Growth Factor 1 Stabilization by Heparin Binding. Journal of Physical Chemistry B, 2021, 125, 12690-12697.	2.6	4
35	Developing a Rational Approach to Designing Recombinant Proteins for Peptide-Directed Nanoparticle Synthesis. Nanoscale Advances, 0, , .	4.6	4
36	An Effective Electric Dipole Model for Voltage-induced Gating Mechanism of Lysenin. Scientific Reports, 2019, 9, 11440.	3.3	3

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37	Mechanistic Picture for Chemomechanical Coupling in a Bacterial Proton-Coupled Oligopeptide Transporter from Streptococcus Thermophilus. Journal of Physical Chemistry B, 2021, 125, 9738-9750.	2.6	2
38	Transient local secondary structure in the intrinsically disordered C-term of the Albino3 insertase. Biophysical Journal, 2021, 120, 4992-5004.	0.5	2
39	Conformational Transition Pathway of GlpT Transporter, Characterized by Nonequilibrium Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 605a-606a.	0.5	0
40	Characterizing Transition Pathways in the Transport Cycle of ABC Transporter MsbA. Biophysical Journal, 2012, 102, 446a.	0.5	0
41	Characterizing the Pathway, Free Energy, and the Effect of Substrate Binding on Structural Transition of MFS Transporter GlpT between Inward- and Outward-Facing States. Biophysical Journal, 2013, 104, 287a.	0.5	0
42	Outward- to Inward-Facing Transition of MsbA Transporter:ÂA Mechanistic Picture at Atomic Resolution. Biophysical Journal, 2013, 104, 288a.	0.5	0
43	Conformational Transition of KcsA Gating and the Mechanism of its pH-Dependence. Biophysical Journal, 2013, 104, 25a.	0.5	0
44	Characterizing the Molecular Mechanism of the Histidine Switch Model in Influenza Virus Hemagglutinin. Biophysical Journal, 2013, 104, 68a.	0.5	0
45	Characterizing Conformational Ensemble and Free Energy Landscape of ABC Exporters using a Novel System-Specific Sampling Approach. Biophysical Journal, 2014, 106, 789a.	0.5	0
46	Driven Adaptive-Bias Scheme: A Hybrid Free Energy Method for Biomolecular Systems with Complex Energy Landscapes. Biophysical Journal, 2014, 106, 640a.	0.5	0
47	Towards Thermodynamic Characterization of Transport Cycle in Secondary Transporters using Enhanced Sampling Techniques. Biophysical Journal, 2015, 108, 144a.	0.5	0
48	Advances in Atomic-Level Simulations of Large-Scale Functional Motions of Membrane Transporters. Biophysical Journal, 2015, 108, 371a.	0.5	0
49	Calculating transition and reaction rates with nonequilibrium work measurements. Journal of Physics: Conference Series, 2015, 640, 012014.	0.4	0