Abhishek Singharoy

List of Publications by Year
in descending order

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50	3,359	331259	223531
papers	citations	21 h-index	46 g-index

60	60	60	4255
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
2	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. Nature Structural and Molecular Biology, 2014, 21, 244-252.	3.6	228
3	Molecular dynamics-based refinement and validation for sub-5 Ã... cryo-electron microscopy maps. ELife, 2016, 5, .	2.8	136
4	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	13.5	122
5	ChAdOx1 interacts with CAR and PF4 with implications for thrombosis with thrombocytopenia syndrome. Science Advances, 2021, 7, eabl8213.	4.7	112
6	Advances in the molecular dynamics flexible fitting method for cryo-EM modeling. Methods, 2016, 100, 50-60.	1.9	82
7	Retrieving functional pathways of biomolecules from single-particle snapshots. Nature Communications, 2020, 11, 4734.	5.8	76
8	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. Nature Methods, 2021, 18, 156-164.	9.0	73
9	Conserved methionine dictates substrate preference in Nramp-family divalent metal transporters. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 10310-10315.	3.3	72
10	A structural model of the active ribosome-bound membrane protein insertase YidC. ELife, 2014, 3, e03035.	2.8	69
11	Computational Methodologies for Real-Space Structural Refinement of Large Macromolecular Complexes. Annual Review of Biophysics, 2016, 45, 253-278.	4.5	67
12	Overall energy conversion efficiency of a photosynthetic vesicle. ELife, 2016, 5, .	2.8	63
13	Crystal Structure and Conformational Change Mechanism of a Bacterial Nramp-Family Divalent Metal Transporter. Structure, 2016, 24, 2102-2114.	1.6	56
14	Flexibility Coexists with Shape-Persistence in Cyanostar Macrocycles. Journal of the American Chemical Society, 2016, 138, 4843-4851.	6.6	53
15	Cryo-EM and MD infer water-mediated proton transport and autoinhibition mechanisms of V _o complex. Science Advances, 2020, 6, .	4.7	51
16	xMDFF: molecular dynamics flexible fitting of low-resolution X-ray structures. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2344-2355.	2.5	50
17	Chemomechanical Coupling in Hexameric Proteinâ€“Protein Interfaces Harnesses Energy within V-Type ATPases. Journal of the American Chemical Society, 2017, 139, 293-310.	6.6	44
18	Atomic detail visualization of photosynthetic membranes with GPU-accelerated ray tracing. Parallel Computing, 2016, 55, 17-27.	1.3	37

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19	Multiscale simulation of microbe structure and dynamics. Progress in Biophysics and Molecular Biology, 2011, 107, 200-217.	1.4	29
20	Macromolecular Crystallography for Synthetic Abiological Molecules: Combining xMDFF and PHENIX for Structure Determination of Cyanostar Macrocycles. Journal of the American Chemical Society, 2015, 137, 8810-8818.	6.6	29
21	CryoFold: Determining protein structures and data-guided ensembles from cryo-EM density maps. Matter, 2021, 4, 3195-3216.	5.0	26
22	The ugly, bad, and good stories of large-scale biomolecular simulations. Current Opinion in Structural Biology, 2022, 73, 102338.	2.6	25
23	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. Journal of Physical Chemistry B, 2017, 121, 3718-3723.	1.2	24
24	Flexible Fitting of Small Molecules into Electron Microscopy Maps Using Molecular Dynamics Simulations with Neural Network Potentials. Journal of Chemical Information and Modeling, 2020, 60, 2591-2604.	2.5	24
25	Charge Transfer and Chemo-Mechanical Coupling in Respiratory Complex I. Journal of the American Chemical Society, 2020, 142, 9220-9230.	6.6	22
26	Methodology for the Simulation of Molecular Motors at Different Scales. Journal of Physical Chemistry B, 2017, 121, 3502-3514.	1.2	20
27	Hydrogen bond network analysis reveals the pathway for the proton transfer in the E-channel of T. thermophilus Complex I. Biochimica Et Biophysica Acta - Bioenergetics, 2020, 1861, 148240.	0.5	20
28	Epitope Fluctuations in the Human Papillomavirus Are Under Dynamic Allosteric Control: A Computational Evaluation of a New Vaccine Design Strategy. Journal of the American Chemical Society, 2013, 135, 18458-18468.	6.6	19
29	Inchworm movement of two rings switching onto a thread by biased Brownian diffusion represent a three-body problem. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9391-9396.	3.3	19
30	Total predicted MHC-I epitope load is inversely associated with population mortality from SARS-CoV-2. Cell Reports Medicine, 2021, 2, 100221.	3.3	17
31	Space Warping Order Parameters and Symmetry: Application to Multiscale Simulation of Macromolecular Assemblies. Journal of Physical Chemistry B, 2012, 116, 8423-8434.	1.2	16
32	Binding Site Recognition and Docking Dynamics of a Single Electron Transport Protein: Cytochrome c₂. Journal of the American Chemical Society, 2016, 138, 12077-12089.	6.6	15
33	Hierarchical Order Parameters for Macromolecular Assembly Simulations. 1. Construction and Dynamical Properties of Order Parameters. Journal of Chemical Theory and Computation, 2012, 8, 1379-1392.	2.3	12
34	Data-guided Multi-Map variables for ensemble refinement of molecular movies. Journal of Chemical Physics, 2020, 153, 214102.	1.2	12
35	Multiscale analytic continuation approach to nanosystem simulation: Applications to virus electrostatics. Journal of Chemical Physics, 2010, 132, 174112.	1.2	10
36	Exploring cryo-electron microscopy with molecular dynamics. Biochemical Society Transactions, 2022, 50, 569-581.	1.6	10

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37	Constructing atomic structural models into cryo-EM densities using molecular dynamics â€“ Pros and cons. Journal of Structural Biology, 2018, 204, 319-328.	1.3	9
38	Mucin-mimetic glycan arrays integrating machine learning for analyzing receptor pattern recognition by influenza A viruses. CheM, 2021, 7, 3393-3411.	5.8	9
39	XFEL and NMR Structures of Francisella Lipoprotein Reveal Conformational Space of Drug Target against Tularemia. Structure, 2020, 28, 540-547.e3.	1.6	8
40	Energy landscape of the SARS-CoV-2 reveals extensive conformational heterogeneity. Current Research in Structural Biology, 2022, 4, 68-77.	1.1	8
41	Rotational Mechanism Model of the Bacterial V1 Motor Based on Structural and Computational Analyses. Frontiers in Physiology, 2019, 10, 46.	1.3	7
42	Molecular Dynamics Flexible Fitting: All You Want to Know About Resolution Exchange. Methods in Molecular Biology, 2020, 2165, 301-315.	0.4	5
43	Anionic Lipids Confine Cytochrome c₂ to the Surface of Bioenergetic Membranes without Compromising Its Interaction with Redox Partners. Biochemistry, 2022, 61, 385-397.	1.2	4
44	Revealing a Hidden Intermediate of Rotatory Catalysis with X-ray Crystallography and Molecular Simulations. ACS Central Science, 2022, 8, 915-925.	5.3	3
45	Large-Scale Molecular Dynamics Simulations of Cellular Compartments. Methods in Molecular Biology, 2021, 2302, 335-356.	0.4	2
46	Antimicrobial Peptide Functionalized Biomaterials Investigated by Molecular Dynamics Simulations. Biophysical Journal, 2020, 118, 380a-381a.	0.2	1
47	Poor Personâ€™s pH Simulation of Membrane Proteins. Methods in Molecular Biology, 2021, 2315, 197-217.	0.4	1
48	New Perspectives on Quinol Binding Motifs at the bc1 Complex Based on MD Simulations. Biophysical Journal, 2015, 108, 602a-603a.	0.2	0
49	Molecular Dynamics Simulations for Improving Crystal Quality and Illuminating the Function of Taspase1: A Therapeutic Target. Biophysical Journal, 2020, 118, 507a.	0.2	0
50	Antimicrobial Peptide-Membrane Interactions: Insights from Molecular Simulations. Biophysical Journal, 2021, 120, 141a.	0.2	0