Yi Wang

List of Publications by Year
in descending order

45 papers	4,854 citations	172457 29 h-index	243625 44 g-index
47 all docs	47 docs citations	47 times ranked	6282 citing authors

#	Article	IF	Citations
1	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
2	Structural mechanism of plant aquaporin gating. Nature, 2006, 439, 688-694.	27.8	752
3	Exploring gas permeability of cellular membranes and membrane channels with molecular dynamics. Journal of Structural Biology, 2007, 157, 534-544.	2.8	184
4	Molecular dynamics simulations of proteins in lipid bilayers. Current Opinion in Structural Biology, 2005, 15, 423-431.	5.7	180
5	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. Journal of Chemical Information and Modeling, 2016, 56, 721-733.	5.4	174
6	What Makes an Aquaporin a Glycerol Channel? A Comparative Study of AqpZ and GlpF. Structure, 2005, 13, 1107-1118.	3.3	159
7	Electrostatic funneling of substrate in mitochondrial inner membrane carriers. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 9598-9603.	7.1	133
8	Implementation of accelerated molecular dynamics in NAMD. Computational Science & Discovery, 2011, 4, 015002.	1.5	124
9	Gaussian Accelerated Molecular Dynamics in NAMD. Journal of Chemical Theory and Computation, 2017, 13, 9-19.	5.3	117
10	Microsecond Molecular Dynamics Simulations of Lipid Mixing. Langmuir, 2014, 30, 11993-12001.	3.5	101
11	Structural and Functional Analysis of SoPIP2;1 Mutants Adds Insight into Plant Aquaporin Gating. Journal of Molecular Biology, 2009, 387, 653-668.	4.2	95
12	Enhanced mechanosensing of cells in synthetic 3D matrix with controlled biophysical dynamics. Nature Communications, 2021, 12, 3514.	12.8	92
13	Accelerating Membrane Simulations with Hydrogen Mass Repartitioning. Journal of Chemical Theory and Computation, 2019, 15, 4673-4686.	5.3	85
14	Nitric oxide conduction by the brain aquaporin AQP4. Proteins: Structure, Function and Bioinformatics, 2010, 78, 661-670.	2.6	84
15	Comparative molecular dynamics simulations of the antimicrobial peptide CM15 in model lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 1402-1409.	2.6	81
16	Identification of triazinoindol-benzimidazolones as nanomolar inhibitors of the Mycobacterium tuberculosis enzyme TDP-6-deoxy-d-xylo-4-hexopyranosid-4-ulose 3,5-epimerase (RmlC). Bioorganic and Medicinal Chemistry, 2010, 18, 896-908.	3.0	79
17	Antimicrobial Peptide Simulations and the Influence of Force Field on the Free Energy for Pore Formation in Lipid Bilayers. Journal of Chemical Theory and Computation, 2016, 12, 4524-4533.	5.3	78
18	Molecular Mechanisms of Conduction and Selectivity in Aquaporin Water Channels. Journal of Nutrition, 2007, 137, 1509S-1515S.	2.9	68

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19	Enhanced Lipid Diffusion and Mixing in Accelerated Molecular Dynamics. Journal of Chemical Theory and Computation, 2011, 7, 3199-3207.	5.3	62
20	Dynamic Conformational States Dictate Selectivity toward the Native Substrate in a Substrate-Permissive Acyltransferase. Biochemistry, 2016, 55, 6314-6326.	2.5	57
21	Tyrosine phosphorylation by Src within the cavity of the adenine nucleotide translocase 1 regulates ADP/ATP exchange in mitochondria. American Journal of Physiology - Cell Physiology, 2010, 298, C740-C748.	4.6	55
22	Selective Permeability of Carboxysome Shell Pores to Anionic Molecules. Journal of Physical Chemistry B, 2018, 122, 9110-9118.	2.6	54
23	Exploring Transmembrane Diffusion Pathways With Molecular Dynamics. Physiology, 2010, 25, 142-154.	3.1	42
24	Effects of histidine protonation and rotameric states on virtual screening of M. tuberculosis RmlC. Journal of Computer-Aided Molecular Design, 2013, 27, 235-246.	2.9	42
25	A Rationally Designed, General Strategy for Membrane Orientation of Photoinduced Electron Transfer-Based Voltage-Sensitive Dyes. ACS Chemical Biology, 2017, 12, 407-413.	3.4	40
26	Estimation of Nanodiamond Surface Charge Density from Zeta Potential and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 3394-3402.	2.6	39
27	Mechanistic basis for the evolution of chalcone synthase catalytic cysteine reactivity in land plants. Journal of Biological Chemistry, 2018, 293, 18601-18612.	3.4	38
28	Spectroscopic and Computational Study of Melittin, Cecropin A, and the Hybrid Peptide CM15. Journal of Physical Chemistry B, 2012, 116, 10600-10608.	2.6	37
29	Link between Membrane Composition and Permeability to Drugs. Journal of Chemical Theory and Computation, 2018, 14, 2895-2909.	5.3	35
30	Anchored but not internalized: shape dependent endocytosis of nanodiamond. Scientific Reports, 2017, 7, 46462.	3.3	31
31	Affordable Membrane Permeability Calculations: Permeation of Short-Chain Alcohols through Pure-Lipid Bilayers and a Mammalian Cell Membrane. Journal of Chemical Theory and Computation, 2019, 15, 2913-2924.	5.3	27
32	Structural and dynamic basis of substrate permissiveness in hydroxycinnamoyltransferase (HCT). PLoS Computational Biology, 2018, 14, e1006511.	3.2	25
33	Free Energy Calculation of Nanodiamond-Membrane Associationâ€”The Effect of Shape and Surface Functionalization. Journal of Chemical Theory and Computation, 2014, 10, 2751-2758.	5.3	24
34	Novel inhibitors of Mycobacterium tuberculosis dTDP-6-deoxy-l-lyxo-4-hexulose reductase (RmlD) identified by virtual screening. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 7064-7067.	2.2	23
35	Effects of Biomolecular Flexibility on Alchemical Calculations of Absolute Binding Free Energies. Journal of Chemical Theory and Computation, 2011, 7, 2224-2232.	5.3	18
36	Chapter 12 Gas Conduction of Lipid Bilayers and Membrane Channels. Current Topics in Membranes, 2008, 60, 343-367.	0.9	12

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37	Structureâ€based network analysis of an evolved G proteinâ€coupled receptor homodimer interface. Protein Science, 2013, 22, 745-754.	7.6	11
38	Investigation of the conformational dynamics of the apo A_{2A} adenosine receptor. Protein Science, 2015, 24, 1004-1012.	7.6	11
39	Independent-Trajectory Thermodynamic Integration: A Practical Guide to Protein-Drug Binding Free Energy Calculations Using Distributed Computing. Methods in Molecular Biology, 2012, 819, 469-486.	0.9	10
40	Pore formation induced by nanoparticles binding to a lipid membrane. Nanoscale, 2020, 12, 7902-7913.	5.6	7
41	Reverse Binding Mode of Phosphotyrosine Peptides with SH2 Protein. Biochemistry, 2018, 57, 5257-5269.	2.5	6
42	Introduction to Molecular Dynamics: Theory and Applications in Biomolecular Modeling. Biological and Medical Physics Series, 2012, , 3-30.	0.4	4
43	Accelerated molecular dynamics: Theory, implementation and applications. , 2012, , .		4
44	Virtual substitution scan via singleâ€step free energy perturbation. Biopolymers, 2016, 105, 324-336.	2.4	3
45	The role of intramolecular nonbonded interaction and angle sampling in single-step free energy perturbation. Journal of Chemical Physics, 2016, 145, 234109.	3.0	1