Fangqiang Zhu

List of Publications by Year
in descending order

32 papers	1,739 citations	516710 16 h-index	454955 30 g-index
32 all docs	32 docs citations	32 times ranked	2112 citing authors

#	Article	IF	Citations
1	Theory and Simulation of Water Permeation in Aquaporin-1. Biophysical Journal, 2004, 86, 50-57.	0.5	332
2	Water and Proton Conduction through Carbon Nanotubes as Models for Biological Channels. Biophysical Journal, 2003, 85, 236-244.	0.5	275
3	Collective Diffusion Model for Water Permeation through Microscopic Channels. Physical Review Letters, 2004, 93, 224501.	7.8	204
4	Convergence and error estimation in free energy calculations using the weighted histogram analysis method. Journal of Computational Chemistry, 2012, 33, 453-465.	3.3	187
5	Pore opening and closing of a pentameric ligand-gated ion channel. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 19814-19819.	7.1	145
6	Drying Transition in the Hydrophobic Gate of the GLIC Channel Blocks Ion Conduction. Biophysical Journal, 2012, 103, 219-227.	0.5	94
7	Water Transport through Nanotubes with Varying Interaction Strength between Tube Wall and Water. Journal of Physical Chemistry Letters, 2011, 2, 2978-2983.	4.6	90
8	Theory and Simulation of Ion Conduction in the Pentameric GLIC Channel. Journal of Chemical Theory and Computation, 2012, 8, 3759-3768.	5.3	62
9	Binding Affinity Prediction by Pairwise Function Based on Neural Network. Journal of Chemical Information and Modeling, 2020, 60, 2766-2772.	5.4	39
10	Gating Transition of Pentameric Ligand-Gated Ion Channels. Biophysical Journal, 2009, 97, 2456-2463.	0.5	35
11	True-color real-time imaging and spectroscopy of carbon nanotubes on substrates using enhanced Rayleigh scattering. Nano Research, 2015, 8, 2721-2732.	10.4	34
12	Mechanism of polymorphism and curvature of HIV capsid assemblies probed by 3D simulations with a novel coarse grain model. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 2353-2367.	2.4	32
13	Conformational Dynamics of a Ligand-Free Adenylate Kinase. PLoS ONE, 2013, 8, e68023.	2.5	27
14	Discovery of Small-Molecule Inhibitors of SARS-CoV-2 Proteins Using a Computational and Experimental Pipeline. Frontiers in Molecular Biosciences, 2021, 8, 678701.	3.5	22
15	Thermodynamics of Protein Folding Studied by Umbrella Sampling along a Reaction Coordinate of Native Contacts. Journal of Chemical Theory and Computation, 2017, 13, 2086-2097.	5.3	20
16	Collective Diffusion Model for Ion Conduction through Microscopic Channels. Biophysical Journal, 2013, 104, 368-376.	0.5	18
17	Finite Temperature String Method with Umbrella Sampling: Application on a Side Chain Flipping in Mhp1 Transporter. Journal of Physical Chemistry B, 2017, 121, 3376-3386.	2.6	14
18	Interface dipole enhancement effect and enhanced Rayleigh scattering. Nano Research, 2015, 8, 303-319.	10.4	12

#	Article	IF	Citations
19	Conformational Changes in Two Inter-Helical Loops of Mhp1 Membrane Transporter. PLoS ONE, 2015, 10, e0133388.	2.5	11
20	Monte Carlo Simulations of HIV Capsid Protein Homodimer. Journal of Chemical Information and Modeling, 2015, 55, 1361-1368.	5.4	11
21	Structural Model of the Tubular Assembly of the Rous Sarcoma Virus Capsid Protein. Journal of the American Chemical Society, 2017, 139, 2006-2013.	13.7	10
22	Calculating Single-Channel Permeability and Conductance from Transition Paths. Journal of Chemical Information and Modeling, 2019, 59, 777-785.	5.4	10
23	Assessing the Perturbing Effects of Drugs on Lipid Bilayers Using Gramicidin Channel-Based In Silico and In Vitro Assays. Journal of Medicinal Chemistry, 2020, 63, 11809-11818.	6.4	10
24	Construction of a novel coarse grain model for simulations of HIV capsid assembly to capture the backbone structure and inter-domain motions in solution. Data in Brief, 2015, 5, 506-512.	1.0	9
25	Vitamin E Has Reduced Affinity for a Polyunsaturated Phospholipid: An Umbrella Sampling Molecular Dynamics Simulations Study. Journal of Physical Chemistry B, 2018, 122, 8351-8358.	2.6	9
26	High-throughput virtual screening of small molecule inhibitors for SARS-CoV-2 protein targets with deep fusion models. , 2021, , .		7
27	Calculating transition rates from durations of transition paths. Journal of Chemical Physics, 2017, 146, 124128.	3.0	5
28	Kinetic mechanism for water in vibrating carbon nanotubes. Physical Review E, 2018, 98, .	2.1	5
29	How does Water Pass through a Sugar Transporter?. Biophysical Journal, 2014, 106, 1229-1230.	0.5	4
30	Parameter Optimization for Interaction between C-Terminal Domains of HIV-1 Capsid Protein. Journal of Chemical Information and Modeling, 2017, 57, 1134-1141.	5.4	3
31	Toward Convergence in Free Energy Calculations for Protein Conformational Changes: A Case Study on the Thin Gate of Mhp1 Transporter. Journal of Chemical Theory and Computation, 2021, 17, 6583-6596.	5.3	3
32	Evaluating membrane affinity by integrating protein orientations. Journal of Molecular Graphics and Modelling, 2014, 54, 141-147.	2.4	0