

Junchao Xia

List of Publications by Year in descending order

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33
papers

755
citations

430874

18
h-index

552781

26
g-index

34
all docs

34
docs citations

34
times ranked

914
citing authors

#	ARTICLE	IF	CITATIONS
1	How Does Water Affect the Dynamics of the Room-Temperature Ionic Liquid 1-Hexyl-3-methylimidazolium Hexafluorophosphate and the Fluorescence Spectroscopy of Coumarin-153 When Dissolved in It?. <i>Journal of Physical Chemistry B</i> , 2008, 112, 1770-1776.	2.6	73
2	The cooling rate dependence of crystallization for liquid copper: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2001, 114, 7506-7512.	3.0	57
3	Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8289-8301.	2.6	42
4	Asynchronous replica exchange software for grid and heterogeneous computing. <i>Computer Physics Communications</i> , 2015, 196, 236-246.	7.5	35
5	Comparing alchemical and physical pathway methods for computing the absolute binding free energy of charged ligands. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17081-17092.	2.8	34
6	Cooling rate dependence of structural properties of aluminium during rapid solidification. <i>Journal of Physics Condensed Matter</i> , 2001, 13, 1873-1890.	1.8	31
7	Sugar Folding: A Novel Structural Prediction Tool for Oligosaccharides and Polysaccharides 2. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1629-1643.	5.3	30
8	Simulation of the Burridge-Knopoff Model of Earthquakes with Variable Range Stress Transfer. <i>Physical Review Letters</i> , 2005, 95, 248501.	7.8	29
9	Sucrose in aqueous solution revisited, Part 1: Molecular dynamics simulations and direct and indirect dipolar coupling analysis. <i>Biopolymers</i> , 2012, 97, 276-288.	2.4	28
10	NMR Relaxation in Proteins with Fast Internal Motions and Slow Conformational Exchange: Model-Free Framework and Markov State Simulations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 6625-6634.	2.6	28
11	When Sugars Get Wet. A Comprehensive Study of the Behavior of Water on the Surface of Oligosaccharides. <i>Journal of Physical Chemistry B</i> , 2009, 113, 11003-11015.	2.6	27
12	A Stochastic Solution to the Unbinned WHAM Equations. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3834-3840.	4.6	27
13	Diffusion and Residence Time of Hydrogen Peroxide and Water in Crowded Protein Environments. <i>Journal of Physical Chemistry B</i> , 2007, 111, 13336-13344.	2.6	26
14	Near-mean-field behavior in the generalized Burridge-Knopoff earthquake model with variable-range stress transfer. <i>Physical Review E</i> , 2008, 77, 031132.	2.1	26
15	A tool for the prediction of structures of complex sugars. <i>Journal of Biomolecular NMR</i> , 2008, 42, 241-256.	2.8	23
16	Molecular Dynamics of the Proline Switch and Its Role in Crk Signaling. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4535-4545.	2.6	21
17	Large-scale asynchronous and distributed multidimensional replica exchange molecular simulations and efficiency analysis. <i>Journal of Computational Chemistry</i> , 2015, 36, 1772-1785.	3.3	19
18	Molecular dynamics simulation of the local inherent structure of liquid silicon at different temperatures. <i>Physical Review B</i> , 1999, 60, 3194-3199.	3.2	18

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19	Searching and Optimizing Structure Ensembles for Complex Flexible Sugars. <i>Journal of the American Chemical Society</i> , 2011, 133, 15252-15255.	13.7	18
20	A combined treatment of hydration and dynamical effects for the modeling of host-guest binding thermodynamics: the SAMPL5 blinded challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 29-44.	2.9	18
21	Sugar Folding: A Novel Structural Prediction Tool for Oligosaccharides and Polysaccharides 1. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1620-1628.	5.3	17
22	Large scale free energy calculations for blind predictions of protein-ligand binding: the D3R Grand Challenge 2015. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 743-751.	2.9	17
23	Locally weighted histogram analysis and stochastic solution for large-scale multi-state free energy estimation. <i>Journal of Chemical Physics</i> , 2016, 144, 034107.	3.0	16
24	Different Cooling Rate Dependences of Different Microstructure Units in Aluminium Glass by Molecular Dynamics Simulation. <i>Chinese Physics Letters</i> , 2000, 17, 34-36.	3.3	14
25	Sucrose in aqueous solution revisited, Part 2: Adaptively biased molecular dynamics simulations and computational analysis of NMR relaxation. <i>Biopolymers</i> , 2012, 97, 289-302.	2.4	14
26	Enhanced Sampling of Interdomain Motion Using Map-Restrained Langevin Dynamics and NMR: Application to Pin1. <i>Journal of Molecular Biology</i> , 2018, 430, 2164-2180.	4.2	12
27	Measuring the magnitude of internal motion in a complex hexasaccharide. <i>Biopolymers</i> , 2011, 95, 39-50.	2.4	11
28	Binding Energy Distribution Analysis Method: Hamiltonian Replica Exchange with Torsional Flattening for Binding Mode Prediction and Binding Free Energy Estimation. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2459-2470.	5.3	11
29	Computational Study of the Conformational Structures of Saccharides in Solution Based on J Couplings and the "Fast Sugar Structure Prediction Software". <i>Biomacromolecules</i> , 2009, 10, 3081-3088.	5.4	9
30	Final Structures of Crystallization of Liquid Copper Studied by Molecular Dynamics Simulation. <i>Chinese Physics Letters</i> , 1999, 16, 850-852.	3.3	8
31	Improving Prediction Accuracy of Binding Free Energies and Poses of HIV Integrase Complexes Using the Binding Energy Distribution Analysis Method with Flattening Potentials. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1356-1371.	5.4	7
32	Massive-Scale Binding Free Energy Simulations of HIV Integrase Complexes Using Asynchronous Replica Exchange Framework Implemented on the IBM WCG Distributed Network. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1382-1397.	5.4	6
33	MODELS OF EARTHQUAKE FAULTS: ERGODICITY AND FORECASTING. <i>International Journal of Modern Physics B</i> , 2009, 23, 5553-5569.	2.0	2