Junchao Xia

List of Publications by Year
in descending order

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33	755	430874	552781
papers	citations	18	26
		h-index	g-index

34	34	34	914
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Massive-Scale Binding Free Energy Simulations of HIV Integrase Complexes Using Asynchronous Replica Exchange Framework Implemented on the IBM WCG Distributed Network. Journal of Chemical Information and Modeling, 2019, 59, 1382-1397.	5.4	6
2	Comparing alchemical and physical pathway methods for computing the absolute binding free energy of charged ligands. Physical Chemistry Chemical Physics, 2018, 20, 17081-17092.	2.8	34
3	Enhanced Sampling of Interdomain Motion Using Map-Restrained Langevin Dynamics and NMR: Application to Pin1. Journal of Molecular Biology, 2018, 430, 2164-2180.	4.2	12
4	Improving Prediction Accuracy of Binding Free Energies and Poses of HIV Integrase Complexes Using the Binding Energy Distribution Analysis Method with Flattening Potentials. Journal of Chemical Information and Modeling, 2018, 58, 1356-1371.	5.4	7
5	A combined treatment of hydration and dynamical effects for the modeling of hostâ€“guest binding thermodynamics: the SAMPL5 blinded challenge. Journal of Computer-Aided Molecular Design, 2017, 31, 29-44.	2.9	18
6	Locally weighted histogram analysis and stochastic solution for large-scale multi-state free energy estimation. Journal of Chemical Physics, 2016, 144, 034107.	3.0	16
7	Binding Energy Distribution Analysis Method: Hamiltonian Replica Exchange with Torsional Flattening for Binding Mode Prediction and Binding Free Energy Estimation. Journal of Chemical Theory and Computation, 2016, 12, 2459-2470.	5.3	11
8	Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit. Journal of Physical Chemistry B, 2016, 120, 8289-8301.	2.6	42
9	Large scale free energy calculations for blind predictions of proteinâ€“ligand binding: the D3R Grand Challenge 2015. Journal of Computer-Aided Molecular Design, 2016, 30, 743-751.	2.9	17
10	Largeâ€scale asynchronous and distributed multidimensional replica exchange molecular simulations and efficiency analysis. Journal of Computational Chemistry, 2015, 36, 1772-1785.	3.3	19
11	Asynchronous replica exchange software for grid and heterogeneous computing. Computer Physics Communications, 2015, 196, 236-246.	7.5	35
12	A Stochastic Solution to the Unbinned WHAM Equations. Journal of Physical Chemistry Letters, 2015, 6, 3834-3840.	4.6	27
13	Molecular Dynamics of the Proline Switch and Its Role in Crk Signaling. Journal of Physical Chemistry B, 2014, 118, 4535-4545.	2.6	21
14	NMR Relaxation in Proteins with Fast Internal Motions and Slow Conformational Exchange: Model-Free Framework and Markov State Simulations. Journal of Physical Chemistry B, 2013, 117, 6625-6634.	2.6	28
15	Sucrose in aqueous solution revisited, Part 2: Adaptively biased molecular dynamics simulations and computational analysis of NMR relaxation. Biopolymers, 2012, 97, 289-302.	2.4	14
16	Sucrose in aqueous solution revisited, Part 1: Molecular dynamics simulations and direct and indirect dipolar coupling analysis. Biopolymers, 2012, 97, 276-288.	2.4	28
17	Searching and Optimizing Structure Ensembles for Complex Flexible Sugars. Journal of the American Chemical Society, 2011, 133, 15252-15255.	13.7	18
18	Measuring the magnitude of internal motion in a complex hexasaccharide. Biopolymers, 2011, 95, 39-50.	2.4	11

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19	MODELS OF EARTHQUAKE FAULTS: ERGODICITY AND FORECASTING. International Journal of Modern Physics B, 2009, 23, 5553-5569.	2.0	2
20	Computational Study of the Conformational Structures of Saccharides in Solution Based on J Couplings and the â€œFast Sugar Structure Prediction Softwareâ€• Biomacromolecules, 2009, 10, 3081-3088.	5.4	9
21	When Sugars Get Wet. A Comprehensive Study of the Behavior of Water on the Surface of Oligosaccharides. Journal of Physical Chemistry B, 2009, 113, 11003-11015.	2.6	27
22	A tool for the prediction of structures of complex sugars. Journal of Biomolecular NMR, 2008, 42, 241-256.	2.8	23
23	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?. Journal of Physical Chemistry B, 2008, 112, 1770-1776.	2.6	73
24	Near-mean-field behavior in the generalized Burridge-Knopoff earthquake model with variable-range stress transfer. Physical Review E, 2008, 77, 031132.	2.1	26
25	Sugar Folding:â€‰ A Novel Structural Prediction Tool for Oligosaccharides and Polysaccharides 1. Journal of Chemical Theory and Computation, 2007, 3, 1620-1628.	5.3	17
26	Sugar Folding:â€‰ A Novel Structural Prediction Tool for Oligosaccharides and Polysaccharides 2. Journal of Chemical Theory and Computation, 2007, 3, 1629-1643.	5.3	30
27	Diffusion and Residence Time of Hydrogen Peroxide and Water in Crowded Protein Environments. Journal of Physical Chemistry B, 2007, 111, 13336-13344.	2.6	26
28	Simulation of the Burridge-Knopoff Model of Earthquakes with Variable Range Stress Transfer. Physical Review Letters, 2005, 95, 248501.	7.8	29
29	The cooling rate dependence of crystallization for liquid copper: A molecular dynamics study. Journal of Chemical Physics, 2001, 114, 7506-7512.	3.0	57
30	Cooling rate dependence of structural properties of aluminium during rapid solidification. Journal of Physics Condensed Matter, 2001, 13, 1873-1890.	1.8	31
31	Different Cooling Rate Dependences of Different Microstructure Units in Aluminium Glass by Molecular Dynamics Simulation. Chinese Physics Letters, 2000, 17, 34-36.	3.3	14
32	Final Structures of Crystallization of Liquid Copper Studied by Molecular Dynamics Simulation. Chinese Physics Letters, 1999, 16, 850-852.	3.3	8
33	Molecular dynamics simulation of the local inherent structure of liquid silicon at different temperatures. Physical Review B, 1999, 60, 3194-3199.	3.2	18