Xiongwu Wu

List of Publications by Year in descending order

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52 papers	2,798 citations	185998 28 h-index	197535 49 g-index
52 all docs	52 docs citations	52 times ranked	3535 citing authors

#	Article	IF	Citations
1	Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. Journal of Chemical Theory and Computation, 2021, 17, 1086-1097.	2.3	16
2	Protonation state of the selectivity filter of bacterial voltageâ€gated sodium channels is modulated by ions. Proteins: Structure, Function and Bioinformatics, 2020, 88, 527-539.	1.5	8
3	Reformulation of the self-guided molecular simulation method. Journal of Chemical Physics, 2020, 153, 094112.	1.2	2
4	The homogeneity condition: A simple way to derive isotropic periodic sum potentials for efficient calculation of long-range interactions in molecular simulation. Journal of Chemical Physics, 2019, 150, 214109.	1.2	5
5	A double exponential potential for van der Waals interaction. AIP Advances, 2019, 9, 065304.	0.6	11
6	Comparison of the umbrella sampling and the double decoupling method in binding free energy predictions for SAMPL6 octa-acid hostâ€“guest challenges. Journal of Computer-Aided Molecular Design, 2018, 32, 1075-1086.	1.3	18
7	Hydronium Ions Accompanying Buried Acidic Residues Lead to High Apparent Dielectric Constants in the Interior of Proteins. Journal of Physical Chemistry B, 2018, 122, 6215-6223.	1.2	6
8	Atomic Resolution Cryo-EM Structure of Î²-Galactosidase. Structure, 2018, 26, 848-856.e3.	1.6	115
9	Origin of pK_a Shifts of Internal Lysine Residues in SNase Studied Via Equal-Molar VMMS Simulations in Explicit Water. Journal of Physical Chemistry B, 2017, 121, 3318-3330.	1.2	18
10	Structure and Dynamics of Macromolecular Assemblies from Electron Microscopy Maps. , 2016, , .		1
11	Isotropic periodic sum for multipole interactions and a vector relation for calculation of the Cartesian multipole tensor. Journal of Chemical Physics, 2016, 145, 164110.	1.2	6
12	Selfâ€guided <scp>L</scp>angevin dynamics via generalized <scp>L</scp>angevin equation. Journal of Computational Chemistry, 2016, 37, 595-601.	1.5	60
13	The ubiquitin ligase Ubr4 controls stability of podocin/MEC-2 supercomplexes. Human Molecular Genetics, 2016, 25, 1328-1344.	1.4	45
14	Maturation of the HIV-1 core by a non-diffusional phase transition. Nature Communications, 2015, 6, 5854.	5.8	49
15	2.2 Ã... resolution cryo-EM structure of Î²-galactosidase in complex with a cell-permeant inhibitor. Science, 2015, 348, 1147-1151.	6.0	440
16	A Virtual Mixture Approach to the Study of Multistate Equilibrium: Application to Constant pH Simulation in Explicit Water. PLoS Computational Biology, 2015, 11, e1004480.	1.5	14
17	Phosphoproteomic Analysis Reveals Regulatory Mechanisms at the Kidney Filtration Barrier. Journal of the American Society of Nephrology: JASN, 2014, 25, 1509-1522.	3.0	40
18	Accurate High-Throughput Structure Mapping and Prediction with Transition Metal Ion FRET. Structure, 2013, 21, 9-19.	1.6	31

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19	Targeted conformational search with map-restrained self-guided Langevin dynamics: Application to flexible fitting into electron microscopic density maps. Journal of Structural Biology, 2013, 183, 429-440.	1.3	50
20	Proteinâ€“Protein Docking Using EMAP in CHARMM and Support Vector Machine: Application to Ab/Ag Complexes. Journal of Chemical Theory and Computation, 2013, 9, 4186-4194.	2.3	6
21	A Common Molecular Basis for Exogenous and Endogenous Cannabinoid Potentiation of Glycine Receptors. Journal of Neuroscience, 2012, 32, 5200-5208.	1.7	53
22	Maintain rigid structures in Verlet based Cartesian molecular dynamics simulations. Journal of Chemical Physics, 2012, 137, 134110.	1.2	17
23	Enhanced Sampling in Free Energy Calculations: Combining SGLD with the Bennettâ€™s Acceptance Ratio and Enveloping Distribution Sampling Methods. Journal of Chemical Theory and Computation, 2012, 8, 3650-3662.	2.3	18
24	Replica exchanging self-guided Langevin dynamics for efficient and accurate conformational sampling. Journal of Chemical Physics, 2012, 137, 044106.	1.2	15
25	Weak Intra-Ring Allosteric Communications of the Archaeal Chaperonin Thermosome Revealed by Normal Mode Analysis. Biophysical Journal, 2012, 103, 1285-1295.	0.2	11
26	Efficient and Unbiased Sampling of Biomolecular Systems in the Canonical Ensemble: A Review of Selfâ€Guided Langevin Dynamics. Advances in Chemical Physics, 2012, 150, 255-326.	0.3	32
27	Toward canonical ensemble distribution from self-guided Langevin dynamics simulation. Journal of Chemical Physics, 2011, 134, 134108.	1.2	37
28	Force-momentum-based self-guided Langevin dynamics: A rapid sampling method that approaches the canonical ensemble. Journal of Chemical Physics, 2011, 135, 204101.	1.2	22
29	Extracellular Complexes of the Hematopoietic Human and Mouse CSF-1 Receptor Are Driven by Common Assembly Principles. Structure, 2011, 19, 1762-1772.	1.6	36
30	Isotropic periodic sum of electrostatic interactions for polar systems. Journal of Chemical Physics, 2009, 131, 024107.	1.2	40
31	Extended Polypeptide Linkers Establish the Spatial Architecture of a Pyruvate Dehydrogenase Multienzyme Complex. Structure, 2008, 16, 93-103.	1.6	22
32	Backbone Relaxation Coupled to the Ionization of Internal Groups in Proteins: A Self-Guided Langevin Dynamics Study. Biophysical Journal, 2008, 95, 4091-4101.	0.2	49
33	Chemoreceptors in Caulobacter crescentus : Trimers of Receptor Dimers in a Partially Ordered Hexagonally Packed Array. Journal of Bacteriology, 2008, 190, 6805-6810.	1.0	72
34	Role of HAMP domains in chemotaxis signaling by bacterial chemoreceptors. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 16555-16560.	3.3	72
35	Using the isotropic periodic sum method to calculate long-range interactions of heterogeneous systems. Journal of Chemical Physics, 2008, 129, 154115.	1.2	58
36	Long-Range Lennard-Jones and Electrostatic Interactions in Interfaces:Â Application of the Isotropic Periodic Sum Method. Journal of Physical Chemistry B, 2007, 111, 4393-4400.	1.2	78

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37	Mutagenesis and Modeling of the Peroxiredoxin (Prx) Complex with the NMR Structure of ATP-Bound Human Sulfiredoxin Implicate Aspartate 187 of Prx I as the Catalytic Residue in ATP Hydrolysisâ€¡. Biochemistry, 2006, 45, 15301-15309.	1.2	21
38	Molecular Structure of a 9-MDa Icosahedral Pyruvate Dehydrogenase Subcomplex Containing the E2 and E3 Enzymes Using Cryoelectron Microscopy. Journal of Biological Chemistry, 2006, 281, 4364-4370.	1.6	72
39	Isotropic periodic sum: A method for the calculation of long-range interactions. Journal of Chemical Physics, 2005, 122, 044107.	1.2	127
40	Î²-Hairpin Folding Mechanism of a Nine-Residue Peptide Revealed from Molecular Dynamics Simulations in Explicit Water. Biophysical Journal, 2004, 86, 1946-1958.	0.2	40
41	The Local Maximum Clustering Method and Its Application in Microarray Gene Expression Data Analysis. Eurasip Journal on Advances in Signal Processing, 2004, 2004, 1.	1.0	24
42	Self-guided Langevin dynamics simulation method. Chemical Physics Letters, 2003, 381, 512-518.	1.2	398
43	A core-weighted fitting method for docking atomic structures into low-resolution maps: Application to cryo-electron microscopy. Journal of Structural Biology, 2003, 141, 63-76.	1.3	77
44	Competitive and Reversible Binding of a Guest Molecule to Its Host in Aqueous Solution through Molecular Dynamics Simulation:Â Benzyl Alcohol/Î²-Cyclodextrin System. Journal of Physical Chemistry B, 2002, 106, 4863-4872.	1.2	40
45	Direct Observation of the Folding and Unfolding of a Î²-Hairpin in Explicit Water through Computer Simulation. Journal of the American Chemical Society, 2002, 124, 5282-5283.	6.6	63
46	Molecular architecture and mechanism of an icosahedral pyruvate dehydrogenase complex: a multifunctional catalytic machine. EMBO Journal, 2002, 21, 5587-5598.	3.5	115
47	Helix Folding of an Alanine-Based Peptide in Explicit Water. Journal of Physical Chemistry B, 2001, 105, 2227-2235.	1.2	51
48	Folding Studies of a Linear Pentamer Peptide Adopting a Reverse Turn Conformation in Aqueous Solution through Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2000, 104, 8023-8034.	1.2	28
49	Enhancing systematic motion in molecular dynamics simulation. Journal of Chemical Physics, 1999, 110, 9401-9410.	1.2	61
50	Self-Guided Molecular Dynamics Simulation for Efficient Conformational Search. Journal of Physical Chemistry B, 1998, 102, 7238-7250.	1.2	108
51	Molecular Simulation with Discrete Fast Fourier Transform. , 0, , .		0
52	Protein-Protein Docking Using Map Objects. , 0, , .		0