

# Xiongwu Wu

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7125435/publications.pdf>

Version: 2024-02-01

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	2.2 Å... resolution cryo-EM structure of Î²-galactosidase in complex with a cell-permeant inhibitor. <i>Science</i> , 2015, 348, 1147-1151.	6.0	440
2	Self-guided Langevin dynamics simulation method. <i>Chemical Physics Letters</i> , 2003, 381, 512-518.	1.2	398
3	Isotropic periodic sum: A method for the calculation of long-range interactions. <i>Journal of Chemical Physics</i> , 2005, 122, 044107.	1.2	127
4	Molecular architecture and mechanism of an icosahedral pyruvate dehydrogenase complex: a multifunctional catalytic machine. <i>EMBO Journal</i> , 2002, 21, 5587-5598.	3.5	115
5	Atomic Resolution Cryo-EM Structure of Î²-Galactosidase. <i>Structure</i> , 2018, 26, 848-856.e3.	1.6	115
6	Self-Guided Molecular Dynamics Simulation for Efficient Conformational Search. <i>Journal of Physical Chemistry B</i> , 1998, 102, 7238-7250.	1.2	108
7	Long-Range Lennard-Jones and Electrostatic Interactions in Interfaces:Â Application of the Isotropic Periodic Sum Method. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4393-4400.	1.2	78
8	A core-weighted fitting method for docking atomic structures into low-resolution maps: Application to cryo-electron microscopy. <i>Journal of Structural Biology</i> , 2003, 141, 63-76.	1.3	77
9	Molecular Structure of a 9-MDa Icosahedral Pyruvate Dehydrogenase Subcomplex Containing the E2 and E3 Enzymes Using Cryoelectron Microscopy. <i>Journal of Biological Chemistry</i> , 2006, 281, 4364-4370.	1.6	72
10	Chemoreceptors in <i>Caulobacter crescentus</i> : Trimers of Receptor Dimers in a Partially Ordered Hexagonally Packed Array. <i>Journal of Bacteriology</i> , 2008, 190, 6805-6810.	1.0	72
11	Role of HAMP domains in chemotaxis signaling by bacterial chemoreceptors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 16555-16560.	3.3	72
12	Direct Observation of the Folding and Unfolding of a Î²-Hairpin in Explicit Water through Computer Simulation. <i>Journal of the American Chemical Society</i> , 2002, 124, 5282-5283.	6.6	63
13	Enhancing systematic motion in molecular dynamics simulation. <i>Journal of Chemical Physics</i> , 1999, 110, 9401-9410.	1.2	61
14	Self-guided Langevin dynamics via generalized Langevin equation. <i>Journal of Computational Chemistry</i> , 2016, 37, 595-601.	1.5	60
15	Using the isotropic periodic sum method to calculate long-range interactions of heterogeneous systems. <i>Journal of Chemical Physics</i> , 2008, 129, 154115.	1.2	58
16	A Common Molecular Basis for Exogenous and Endogenous Cannabinoid Potentiation of Glycine Receptors. <i>Journal of Neuroscience</i> , 2012, 32, 5200-5208.	1.7	53
17	Helix Folding of an Alanine-Based Peptide in Explicit Water. <i>Journal of Physical Chemistry B</i> , 2001, 105, 2227-2235.	1.2	51
18	Targeted conformational search with map-restrained self-guided Langevin dynamics: Application to flexible fitting into electron microscopic density maps. <i>Journal of Structural Biology</i> , 2013, 183, 429-440.	1.3	50

#	ARTICLE	IF	CITATIONS
19	Backbone Relaxation Coupled to the Ionization of Internal Groups in Proteins: A Self-Guided Langevin Dynamics Study. <i>Biophysical Journal</i> , 2008, 95, 4091-4101.	0.2	49
20	Maturation of the HIV-1 core by a non-diffusional phase transition. <i>Nature Communications</i> , 2015, 6, 5854.	5.8	49
21	The ubiquitin ligase Ubr4 controls stability of podocin/MEC-2 supercomplexes. <i>Human Molecular Genetics</i> , 2016, 25, 1328-1344.	1.4	45
22	Competitive and Reversible Binding of a Guest Molecule to Its Host in Aqueous Solution through Molecular Dynamics Simulation: A Benzyl Alcohol/ $\beta$ -Cyclodextrin System. <i>Journal of Physical Chemistry B</i> , 2002, 106, 4863-4872.	1.2	40
23	$\beta$ -Hairpin Folding Mechanism of a Nine-Residue Peptide Revealed from Molecular Dynamics Simulations in Explicit Water. <i>Biophysical Journal</i> , 2004, 86, 1946-1958.	0.2	40
24	Isotropic periodic sum of electrostatic interactions for polar systems. <i>Journal of Chemical Physics</i> , 2009, 131, 024107.	1.2	40
25	Phosphoproteomic Analysis Reveals Regulatory Mechanisms at the Kidney Filtration Barrier. <i>Journal of the American Society of Nephrology: JASN</i> , 2014, 25, 1509-1522.	3.0	40
26	Toward canonical ensemble distribution from self-guided Langevin dynamics simulation. <i>Journal of Chemical Physics</i> , 2011, 134, 134108.	1.2	37
27	Extracellular Complexes of the Hematopoietic Human and Mouse CSF-1 Receptor Are Driven by Common Assembly Principles. <i>Structure</i> , 2011, 19, 1762-1772.	1.6	36
28	Efficient and Unbiased Sampling of Biomolecular Systems in the Canonical Ensemble: A Review of Self-Guided Langevin Dynamics. <i>Advances in Chemical Physics</i> , 2012, 150, 255-326.	0.3	32
29	Accurate High-Throughput Structure Mapping and Prediction with Transition Metal Ion FRET. <i>Structure</i> , 2013, 21, 9-19.	1.6	31
30	Folding Studies of a Linear Pentamer Peptide Adopting a Reverse Turn Conformation in Aqueous Solution through Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2000, 104, 8023-8034.	1.2	28
31	The Local Maximum Clustering Method and Its Application in Microarray Gene Expression Data Analysis. <i>Eurasip Journal on Advances in Signal Processing</i> , 2004, 2004, 1.	1.0	24
32	Extended Polypeptide Linkers Establish the Spatial Architecture of a Pyruvate Dehydrogenase Multienzyme Complex. <i>Structure</i> , 2008, 16, 93-103.	1.6	22
33	Force-momentum-based self-guided Langevin dynamics: A rapid sampling method that approaches the canonical ensemble. <i>Journal of Chemical Physics</i> , 2011, 135, 204101.	1.2	22
34	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 Hydrolysis. <i>Biochemistry</i> , 2006, 45, 15301-15309.	1.2	21
35	Enhanced Sampling in Free Energy Calculations: Combining SGLD with the Bennett's Acceptance Ratio and Enveloping Distribution Sampling Methods. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3650-3662.	2.3	18
36	Origin of pK <sub>a</sub> Shifts of Internal Lysine Residues in SNase Studied Via Equal-Molar VMMS Simulations in Explicit Water. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3318-3330.	1.2	18

#	ARTICLE	IF	CITATIONS
37	Comparison of the umbrella sampling and the double decoupling method in binding free energy predictions for SAMPL6 octa-acid host-guest challenges. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1075-1086.	1.3	18
38	Maintain rigid structures in Verlet based Cartesian molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2012, 137, 134110.	1.2	17
39	Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1086-1097.	2.3	16
40	Replica exchanging self-guided Langevin dynamics for efficient and accurate conformational sampling. <i>Journal of Chemical Physics</i> , 2012, 137, 044106.	1.2	15
41	A Virtual Mixture Approach to the Study of Multistate Equilibrium: Application to Constant pH Simulation in Explicit Water. <i>PLoS Computational Biology</i> , 2015, 11, e1004480.	1.5	14
42	Weak Intra-Ring Allosteric Communications of the Archaeal Chaperonin Thermosome Revealed by Normal Mode Analysis. <i>Biophysical Journal</i> , 2012, 103, 1285-1295.	0.2	11
43	A double exponential potential for van der Waals interaction. <i>AIP Advances</i> , 2019, 9, 065304.	0.6	11
44	Protonation state of the selectivity filter of bacterial voltage-gated sodium channels is modulated by ions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 527-539.	1.5	8
45	Protein-Protein Docking Using EMAP in CHARMM and Support Vector Machine: Application to Ab/Ag Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4186-4194.	2.3	6
46	Isotropic periodic sum for multipole interactions and a vector relation for calculation of the Cartesian multipole tensor. <i>Journal of Chemical Physics</i> , 2016, 145, 164110.	1.2	6
47	Hydronium Ions Accompanying Buried Acidic Residues Lead to High Apparent Dielectric Constants in the Interior of Proteins. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6215-6223.	1.2	6
48	The homogeneity condition: A simple way to derive isotropic periodic sum potentials for efficient calculation of long-range interactions in molecular simulation. <i>Journal of Chemical Physics</i> , 2019, 150, 214109.	1.2	5
49	Reformulation of the self-guided molecular simulation method. <i>Journal of Chemical Physics</i> , 2020, 153, 094112.	1.2	2
50	Structure and Dynamics of Macromolecular Assemblies from Electron Microscopy Maps. , 2016, , .		1
51	Molecular Simulation with Discrete Fast Fourier Transform. , 0, , .		0
52	Protein-Protein Docking Using Map Objects. , 0, , .		0