Wei Han

List of Publications by Year
in descending order

38 papers	1,701 citations	304743 22 h-index	330143 37 g-index
40 all docs	40 docs citations	40 times ranked	2071 citing authors

#	Article	IF	Citations
1	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. Advances in Protein Chemistry and Structural Biology, 2014, 96, 235-265.	2.3	214
2	Fibril Elongation by AÎ²_{17â€“42}: Kinetic Network Analysis of Hybrid-Resolution Molecular Dynamics Simulations. Journal of the American Chemical Society, 2014, 136, 12450-12460.	13.7	127
3	Further Optimization of a Hybrid United-Atom and Coarse-Grained Force Field for Folding Simulations: Improved Backbone Hydration and Interactions between Charged Side Chains. Journal of Chemical Theory and Computation, 2012, 8, 4413-4424.	5.3	120
4	Theoretical Analysis of Secondary Structures of Î²-Peptides. Accounts of Chemical Research, 2008, 41, 1418-1427.	15.6	113
5	Macrolide antibiotics allosterically predispose the ribosome for translation arrest. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 9804-9809.	7.1	99
6	PACE Force Field for Protein Simulations. 1. Full Parameterization of Version 1 and Verification. Journal of Chemical Theory and Computation, 2010, 6, 3373-3389.	5.3	89
7	A Strand-Loop-Strand Structure Is a Possible Intermediate in Fibril Elongation:â€‰ Long Time Simulations of Amyloid-Î² Peptide (10â˜35). Journal of the American Chemical Society, 2005, 127, 15408-15416.	13.7	78
8	Transient Î²-hairpin formation in Î±-synuclein monomer revealed by coarse-grained molecular dynamics simulation. Journal of Chemical Physics, 2015, 143, 243142.	3.0	73
9	Parameterization of PACE Force Field for Membrane Environment and Simulation of Helical Peptides and Helixâ€“Helix Association. Journal of Chemical Theory and Computation, 2012, 8, 300-313.	5.3	61
10	Water access points and hydration pathways in CLC H ⁺ /Cl ^{â˜} transporters. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 1819-1824.	7.1	58
11	The intrinsic conformational features of amino acids from a protein coil library and their applications in force field development. Physical Chemistry Chemical Physics, 2013, 15, 3413.	2.8	55
12	PACE Force Field for Protein Simulations. 2. Folding Simulations of Peptides. Journal of Chemical Theory and Computation, 2010, 6, 3390-3402.	5.3	51
13	CHARMM-GUI PACE CG Builder for Solution, Micelle, and Bilayer Coarse-Grained Simulations. Journal of Chemical Information and Modeling, 2014, 54, 1003-1009.	5.4	47
14	Self-Assembly Pathways of Î²-Sheet-Rich Amyloid-Î²(1â€“40) Dimers: Markov State Model Analysis on Millisecond Hybrid-Resolution Simulations. Journal of Chemical Theory and Computation, 2017, 13, 5731-5744.	5.3	45
15	Conformation Dependence of Diphenylalanine Self-Assembly Structures and Dynamics: Insights from Hybrid-Resolution Simulations. ACS Nano, 2019, 13, 4455-4468.	14.6	45
16	Influence of Side Chain Conformations on Local Conformational Features of Amino Acids and Implication for Force Field Development. Journal of Physical Chemistry B, 2010, 114, 5840-5850.	2.6	44
17	Revealing an outward-facing open conformational state in a CLC Clâ€“/H+ exchange transporter. ELife, 2016, 5, .	6.0	43
18	Coarse-Grained Protein Model Coupled with a Coarse-Grained Water Model:â€‰ Molecular Dynamics Study of Polyalanine-Based Peptides. Journal of Chemical Theory and Computation, 2007, 3, 2146-2161.	5.3	42

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19	Assembly of Nsp1 Nucleoporins Provides Insight into Nuclear Pore Complex Gating. PLoS Computational Biology, 2014, 10, e1003488.	3.2	42
20	Toward a Coarse-Grained Protein Model Coupled with a Coarse-Grained Solvent Model: Solvation Free Energies of Amino Acid Side Chains. Journal of Chemical Theory and Computation, 2008, 4, 1891-1901.	5.3	39
21	Characterization of Folding Mechanisms of Trp-Cage and WW-Domain by Network Analysis of Simulations with a Hybrid-Resolution Model. Journal of Physical Chemistry B, 2013, 117, 13367-13377.	2.6	39
22	Molecular Basis for Differential Anion Binding and Proton Coupling in the Cl^{â€“}/H⁺ Exchanger ClC-ec1. Journal of the American Chemical Society, 2016, 138, 3066-3075.	13.7	36
23	Initial Substrate Binding of Î³-Secretase: The Role of Substrate Flexibility. ACS Chemical Neuroscience, 2017, 8, 1279-1290.	3.5	23
24	Molecular dynamics studies of hexamers of amyloid-Î² peptide (16-35) and its mutants: Influence of charge states on amyloid formation. Proteins: Structure, Function and Bioinformatics, 2006, 66, 575-587.	2.6	22
25	Î±-Helical Motif as Inhibitors of Toxic Amyloid-Î² Oligomer Generation via Highly Specific Recognition of Amyloid Surface. IScience, 2019, 17, 87-100.	4.1	12
26	Computational studies of protein aggregation mediated by amyloid: Fibril elongation and secondary nucleation. Progress in Molecular Biology and Translational Science, 2020, 170, 461-504.	1.7	12
27	Molecular design of stapled pentapeptides as building blocks of self-assembled coiled coilâ€“like fibers. Science Advances, 2021, 7, .	10.3	12
28	Recognition of Poly-Ubiquitins by the Proteasome through Protein Refolding Guided by Electrostatic and Hydrophobic Interactions. Journal of Physical Chemistry B, 2016, 120, 8137-8146.	2.6	11
29	In Silico Study of Recognition between AÎ²₄₀ and AÎ²₄₀ Fibril Surfaces: An N-Terminal Helical Recognition Motif and Its Implications for Inhibitor Design. ACS Chemical Neuroscience, 2018, 9, 935-944.	3.5	11
30	Development of a Hybrid-Resolution Force Field for Peptide Self-Assembly Simulations: Optimizing Peptideâ€“Peptide and Peptideâ€“Solvent Interactions. Journal of Chemical Information and Modeling, 2022, 62, 2744-2760.	5.4	7
31	Parametrization of MARTINI for Modeling Hinging Motions in Membrane Proteins. Journal of Physical Chemistry B, 2019, 123, 2254-2269.	2.6	6
32	Multiscale Exploration of Concentration-Dependent Amyloid-Î²(16-21) Amyloid Nucleation. Journal of Physical Chemistry Letters, 2022, 13, 5009-5016.	4.6	6
33	Targeting the Amyloid-Î² Fibril Surface with a Constrained Helical Peptide Inhibitor. Biochemistry, 2020, 59, 290-296.	2.5	5
34	A Microscopic View of the Mechanisms of Active Transport Across the Cellular Membrane. Annual Reports in Computational Chemistry, 2014, 10, 77-125.	1.7	4
35	Sequence-Dependent Nanofiber Structures of Phenylalanine and Isoleucine Tripeptides. International Journal of Molecular Sciences, 2020, 21, 8431.	4.1	4
36	Bottom-up derived flexible water model with dipole and quadrupole moments for coarse-grained molecular simulations. Physical Chemistry Chemical Physics, 2020, 22, 27394-27412.	2.8	3

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37	Anatomy and formation mechanisms of early amyloid-Î² oligomers with lateral branching: graph network analysis on large-scale simulations. Chemical Science, 2022, 13, 2649-2660.	7.4	3
38	In silico study on the effect of F19T mutation on amyloid-b peptide (10-35). Frontiers in Bioscience - Landmark, 2008, Volume, 3951.	3.0	0