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	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
2	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
3	Multiscale Exploration of Concentration-Dependent Amyloid-Î²(16-21) Amyloid Nucleation. Journal of Physical Chemistry Letters, 2022, 13, 5009-5016.	4.6	6
4	Molecular design of stapled pentapeptides as building blocks of self-assembled coiled coilâ€“like fibers. Science Advances, 2021, 7, .	10.3	12
5	Targeting the Amyloid-Î² Fibril Surface with a Constrained Helical Peptide Inhibitor. Biochemistry, 2020, 59, 290-296.	2.5	5
6	Sequence-Dependent Nanofiber Structures of Phenylalanine and Isoleucine Tripeptides. International Journal of Molecular Sciences, 2020, 21, 8431.	4.1	4
7	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
8	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
9	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
10	Conformation Dependence of Diphenylalanine Self-Assembly Structures and Dynamics: Insights from Hybrid-Resolution Simulations. ACS Nano, 2019, 13, 4455-4468.	14.6	45
11	Parametrization of MARTINI for Modeling Hinging Motions in Membrane Proteins. Journal of Physical Chemistry B, 2019, 123, 2254-2269.	2.6	6
12	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
13	Initial Substrate Binding of Î³-Secretase: The Role of Substrate Flexibility. ACS Chemical Neuroscience, 2017, 8, 1279-1290.	3.5	23
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	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
16	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
17	Revealing an outward-facing open conformational state in a CLC Clâ€“/H+ exchange transporter. ELife, 2016, 5, .	6.0	43
18	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

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19	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
20	Assembly of Nsp1 Nucleoporins Provides Insight into Nuclear Pore Complex Gating. PLoS Computational Biology, 2014, 10, e1003488.	3.2	42
21	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
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	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
30	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
31	PACE Force Field for Protein Simulations. 2. Folding Simulations of Peptides. Journal of Chemical Theory and Computation, 2010, 6, 3390-3402.	5.3	51
32	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
33	Theoretical Analysis of Secondary Structures of Î²-Peptides. Accounts of Chemical Research, 2008, 41, 1418-1427.	15.6	113
34	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
35	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
36	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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37	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
38	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