Jianhan Chen

List of Publications by Year
in descending order

82 papers	3,938 citations	126708 33 h-index	128067 60 g-index
90 all docs	90 docs citations	90 times ranked	4183 citing authors

#	Article	IF	Citations
1	Power generation from ambient humidity using protein nanowires. Nature, 2020, 578, 550-554.	13.7	398
2	Balancing Solvation and Intramolecular Interactions:Â Toward a Consistent Generalized Born Force Field. Journal of the American Chemical Society, 2006, 128, 3728-3736.	6.6	327
3	Recent advances in implicit solvent-based methods for biomolecular simulations. Current Opinion in Structural Biology, 2008, 18, 140-148.	2.6	294
4	Bioinspired bio-voltage memristors. Nature Communications, 2020, 11, 1861.	5.8	144
5	Implicit modeling of nonpolar solvation for simulating protein folding and conformational transitions. Physical Chemistry Chemical Physics, 2008, 10, 471-481.	1.3	130
6	Can molecular dynamics simulations provide high-resolution refinement of protein structure?. Proteins: Structure, Function and Bioinformatics, 2007, 67, 922-930.	1.5	124
7	Intrinsic disorder mediates the diverse regulatory functions of the Cdk inhibitor p21. Nature Chemical Biology, 2011, 7, 214-221.	3.9	114
8	Revisiting the Carboxylic Acid Dimers in Aqueous Solution:â€‰ Interplay of Hydrogen Bonding, Hydrophobic Interactions, and Entropy. Journal of Physical Chemistry B, 2008, 112, 242-249.	1.2	103
9	Atomistic Details of the Disordered States of KID and pKID. Implications in Coupled Binding and Folding. Journal of the American Chemical Society, 2009, 131, 5214-5223.	6.6	88
10	Exploring atomistic details of pH-dependent peptide folding. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 18546-18550.	3.3	85
11	Intrinsically Disordered p53 Extreme C-Terminus Binds to S100B(Î²Î²) through â€œFly-Castingâ€. Journal of the American Chemical Society, 2009, 131, 2088-2089.	6.6	84
12	Residual Structures, Conformational Fluctuations, and Electrostatic Interactions in the Synergistic Folding of Two Intrinsically Disordered Proteins. PLoS Computational Biology, 2012, 8, e1002353.	1.5	78
13	EGCG binds intrinsically disordered N-terminal domain of p53 and disrupts p53-MDM2 interaction. Nature Communications, 2021, 12, 986.	5.8	77
14	Towards the physical basis of how intrinsic disorder mediates protein function. Archives of Biochemistry and Biophysics, 2012, 524, 123-131.	1.4	74
15	Electrostatically Accelerated Encounter and Folding for Facile Recognition of Intrinsically Disordered Proteins. PLoS Computational Biology, 2013, 9, e1003363.	1.5	74
16	Electrostatically Accelerated Coupled Binding and Folding of Intrinsically Disordered Proteins. Journal of Molecular Biology, 2012, 422, 674-684.	2.0	71
17	Structural Interpretation of Paramagnetic Relaxation Enhancement-Derived Distances for Disordered Protein States. Journal of Molecular Biology, 2009, 390, 467-477.	2.0	70
18	Hydrophobic gating in BK channels. Nature Communications, 2018, 9, 3408.	5.8	70

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19	Application of torsion angle molecular dynamics for efficient sampling of protein conformations. Journal of Computational Chemistry, 2005, 26, 1565-1578.	1.5	67
20	Topologyâ€based modeling of intrinsically disordered proteins: Balancing intrinsic folding and intermolecular interactions. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1251-1266.	1.5	67
21	Atomistic modelling of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS). Journal of Applied Crystallography, 2016, 49, 1861-1875.	1.9	67
22	Peptide and Protein Folding and Conformational Equilibria: Theoretical Treatment of Electrostatics and Hydrogen Bonding with Implicit Solvent Models. Advances in Protein Chemistry, 2005, 72, 173-198.	4.4	63
23	Molecular basis of PIP2-dependent regulation of the Ca2+-activated chloride channel TMEM16A. Nature Communications, 2019, 10, 3769.	5.8	63
24	Model-free Analysis of Protein Dynamics: Assessment of Accuracy and Model Selection Protocols Based on Molecular Dynamics Simulation. Journal of Biomolecular NMR, 2004, 29, 243-257.	1.6	60
25	Refinement of NMR Structures Using Implicit Solvent and Advanced Sampling Techniques. Journal of the American Chemical Society, 2004, 126, 16038-16047.	6.6	60
26	Synergistic folding of two intrinsically disordered proteins: searching for conformational selection. Molecular BioSystems, 2012, 8, 198-209.	2.9	51
27	An Evaluation of Explicit Receptor Flexibility in Molecular Docking Using Molecular Dynamics and Torsion Angle Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 2909-2923.	2.3	48
28	Intrinsically Disordered Proteins in a Physics-Based World. International Journal of Molecular Sciences, 2010, 11, 5292-5309.	1.8	48
29	An inner activation gate controls TMEM16F phospholipid scrambling. Nature Communications, 2019, 10, 1846.	5.8	47
30	Amyloid assembly is dominated by misregistered kinetic traps on an unbiased energy landscape. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 10322-10328.	3.3	47
31	Accelerate Sampling in Atomistic Energy Landscapes Using Topology-Based Coarse-Grained Models. Journal of Chemical Theory and Computation, 2014, 10, 918-923.	2.3	41
32	Critical Importance of Length-Scale Dependence in Implicit Modeling of Hydrophobic Interactions. Journal of the American Chemical Society, 2007, 129, 2444-2445.	6.6	38
33	Generation of native-like protein structures from limited NMR data, modern force fields and advanced conformational sampling. Journal of Biomolecular NMR, 2005, 31, 59-64.	1.6	36
34	Targeting Intrinsically Disordered Proteins through Dynamic Interactions. Biomolecules, 2020, 10, 743.	1.8	34
35	FoldGPCR: Structure prediction protocol for the transmembrane domain of G proteinâ€coupled receptors from class A. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2189-2201.	1.5	33
36	Modulation of the Disordered Conformational Ensembles of the p53 Transactivation Domain by Cancer-Associated Mutations. PLoS Computational Biology, 2015, 11, e1004247.	1.5	32

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37	Residual Structures and Transient Long-Range Interactions of p53 Transactivation Domain: Assessment of Explicit Solvent Protein Force Fields. Journal of Chemical Theory and Computation, 2019, 15, 4708-4720.	2.3	32
38	Intrinsically Disordered Proteins: Structure, Function and Therapeutics. Journal of Molecular Biology, 2018, 430, 2275-2277.	2.0	30
39	Different Anomeric Sugar Bound States of Maltose Binding Protein Resolved by a Cytolysin A Nanopore Tweezer. ACS Nano, 2020, 14, 1727-1737.	7.3	30
40	Application of solid-state NMR restraint potentials in membrane protein modeling. Journal of Magnetic Resonance, 2008, 193, 68-76.	1.2	29
41	Modulation of Amyloid-Î²42 Conformation by Small Molecules Through Nonspecific Binding. Journal of Chemical Theory and Computation, 2019, 15, 5169-5174.	2.3	28
42	Multiscale filter diagonalization method for spectral analysis of noisy data with nonlocalized features. Journal of Chemical Physics, 2000, 112, 4429-4437.	1.2	27
43	Multiscale enhanced sampling of intrinsically disordered protein conformations. Journal of Computational Chemistry, 2016, 37, 550-557.	1.5	27
44	Efficiency of Adaptive Temperature-Based Replica Exchange for Sampling Large-Scale Protein Conformational Transitions. Journal of Chemical Theory and Computation, 2013, 9, 2849-2856.	2.3	25
45	Potential Conformational Heterogeneity of p53 Bound to S100B(Î²Î²). Journal of Molecular Biology, 2013, 425, 999-1010.	2.0	24
46	Optimization of the GBMV2 implicit solvent force field for accurate simulation of protein conformational equilibria. Journal of Computational Chemistry, 2017, 38, 1332-1341.	1.5	24
47	Residual Structure Accelerates Binding of Intrinsically Disordered ACTR by Promoting Efficient Folding upon Encounter. Journal of Molecular Biology, 2019, 431, 422-432.	2.0	24
48	Effective Approximation of Molecular Volume Using Atom-Centered Dielectric Functions in Generalized Born Models. Journal of Chemical Theory and Computation, 2010, 6, 2790-2803.	2.3	23
49	Hydrophobic dewetting in gating and regulation of transmembrane protein ion channels. Journal of Chemical Physics, 2020, 153, 110901.	1.2	22
50	Branched Oligopeptides Form Nanocapsules with Lipid Vesicle Characteristics. Langmuir, 2013, 29, 14648-14654.	1.6	21
51	Specific PIP2 binding promotes calcium activation of TMEM16A chloride channels. Communications Biology, 2021, 4, 259.	2.0	21
52	HyRes: a coarse-grained model for multi-scale enhanced sampling of disordered protein conformations. Physical Chemistry Chemical Physics, 2017, 19, 32421-32432.	1.3	19
53	Force-Induced Unfolding Simulations of the Human Notch1 Negative Regulatory Region: Possible Roles of the Heterodimerization Domain in Mechanosensing. PLoS ONE, 2011, 6, e22837.	1.1	19
54	MEFA (multiepitope fusion antigen) - Novel Technology for Structural Vaccinology, Proof from Computational and Empirical Immunogenicity Characterization of an Enterotoxigenic Escherichia coli (ETEC) Adhesin MEFA. Journal of Vaccines & Vaccination, 2017, 08, .	0.3	18

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55	Enhanced Sampling of Intrinsic Structural Heterogeneity of the BH3-Only Protein Binding Interface of Bcl-xL. Journal of Physical Chemistry B, 2017, 121, 9160-9168.	1.2	17
56	Advanced Sampling Methods for Multiscale Simulation of Disordered Proteins and Dynamic Interactions. Biomolecules, 2021, 11, 1416.	1.8	17
57	Replica exchange with guided annealing for accelerated sampling of disordered protein conformations. Journal of Computational Chemistry, 2014, 35, 1682-1689.	1.5	14
58	The Levinthal Problem in Amyloid Aggregation: Sampling of a Flat Reaction Space. Journal of Physical Chemistry B, 2017, 121, 1576-1586.	1.2	14
59	Combined Monte Carlo/torsion-angle molecular dynamics for ensemble modeling of proteins, nucleic acids and carbohydrates. Journal of Molecular Graphics and Modelling, 2017, 73, 179-190.	1.3	14
60	Cancer-Associated Mutations Perturb the Disordered Ensemble and Interactions of the Intrinsically Disordered p53 Transactivation Domain. Journal of Molecular Biology, 2021, 433, 167048.	2.0	14
61	Dynamics of the BH3-Only Protein Binding Interface of Bcl-xL. Biophysical Journal, 2015, 109, 1049-1057.	0.2	11
62	Intrinsically Disordered N-terminal Domain (NTD) of p53 Interacts with Mitochondrial PTP Regulator Cyclophilin D. Journal of Molecular Biology, 2022, 434, 167552.	2.0	11
63	Accelerating the Generalized Born with Molecular Volume and Solvent Accessible Surface Area Implicit Solvent Model Using Graphics Processing Units. Journal of Computational Chemistry, 2020, 41, 830-838.	1.5	9
64	Physics-based modeling provides predictive understanding of selectively promiscuous substrate binding by Hsp70 chaperones. PLoS Computational Biology, 2021, 17, e1009567.	1.5	9
65	Necessity of highâ€resolution for coarseâ€grained modeling of flexible proteins. Journal of Computational Chemistry, 2016, 37, 1725-1733.	1.5	8
66	Structural characterization of two poreâ€forming peptides: Consequences of introducing a Câ€terminal tryptophan. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2238-2250.	1.5	7
67	Organization and Structure of Branched Amphipathic Oligopeptide Bilayers. Langmuir, 2016, 32, 9883-9891.	1.6	7
68	Atomistic Peptide Folding Simulations Reveal Interplay of Entropy and Long-Range Interactions in Folding Cooperativity. Scientific Reports, 2018, 8, 13668.	1.6	7
69	Effects of Flanking Loops on Membrane Insertion of Transmembrane Helices: A Role for Peptide Conformational Equilibrium. Journal of Physical Chemistry B, 2013, 117, 8330-8339.	1.2	4
70	Conformational Flexibility and pH Effects on Anisotropic Growth of Sheet-Like Assembly of Amphiphilic Peptides. Journal of Nanoscience and Nanotechnology, 2015, 15, 4470-4479.	0.9	4
71	Modulation of p53 Transactivation Domain Conformations by Ligand Binding and Cancer-Associated Mutations. , 2019, , .		4
72	Modulation of p53 Transactivation Domain Conformations by Ligand Binding and Cancer-Associated Mutations. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2020, 25, 195-206.	0.7	4

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73	Accelerating atomistic simulations of proteins using multiscale enhanced sampling with independent tempering. Journal of Computational Chemistry, 2021, 42, 358-364.	1.5	2
74	Aromatic interactions with membrane modulate human BK channel activation. ELife, 2020, 9, .	2.8	2
75	Computing Energy Levels by Inversion of Imaginary-Time Cross-Correlation Functions. Journal of Physical Chemistry A, 2003, 107, 7175-7180.	1.1	1
76	Implicit Solvent Force-Field Optimization. , 0, , 167-190.		1
77	Free energy analysis of conductivity and charge selectivity of M2GlyR-derived synthetic channels. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2319-2325.	1.4	1
78	Efficacy of independence sampling in replica exchange simulations of ordered and disordered proteins. Journal of Computational Chemistry, 2017, 38, 2632-2640.	1.5	1
79	Positional Isomers of a Non-Nucleoside Substrate Differentially Affect Myosin Function. Biophysical Journal, 2020, 119, 567-580.	0.2	1
80	Expression and Characterization of <i>Manduca sexta</i> Stress Responsive Peptide-1; An Inducer of Antimicrobial Peptide Synthesis. Biochemistry and Molecular Biology, 2019, 4, 42.	0.2	1
81	Atomistic Glimpse of the Orderly Chaos of One Protein. Biophysical Journal, 2015, 109, 1511-1512.	0.2	0
82	INTRINSICALLY DISORDERED PROTEINS: ANALYSIS, PREDICTION, SIMULATION, AND BIOLOGY. , 2011, , .		0