Jianhan Chen

List of Publications by Citations

80 papers	3,011 citations	31 h-index	53 g-index
90 ext. papers	3,486 ext. citations	6.9 avg, IF	5.79 L-index

#	Paper	IF	Citations
80	Balancing solvation and intramolecular interactions: toward a consistent generalized Born force field. *Journal of the American Chemical Society*, **2006**, 128, 3728-36	16.4	290
79	Recent advances in implicit solvent-based methods for biomolecular simulations. *Current Opinion in Structural Biology*, **2008**, 18, 140-8	8.1	266
78	Power generation from ambient humidity using protein nanowires. *Nature*, **2020**, 578, 550-554	50.4	169
77	Can molecular dynamics simulations provide high-resolution refinement of protein structure?. *Proteins: Structure, Function and Bioinformatics*, **2007**, 67, 922-30	4.2	116
76	Implicit modeling of nonpolar solvation for simulating protein folding and conformational transitions. *Physical Chemistry Chemical Physics*, **2008**, 10, 471-81	3.6	116
75	Intrinsic disorder mediates the diverse regulatory functions of the Cdk inhibitor p21. *Nature Chemical Biology*, **2011**, 7, 214-21	11.7	98
74	Atomistic details of the disordered states of KID and pKID. Implications in coupled binding and folding. *Journal of the American Chemical Society*, **2009**, 131, 5214-23	16.4	82
73	Revisiting the carboxylic acid dimers in aqueous solution: interplay of hydrogen bonding, hydrophobic interactions, and entropy. *Journal of Physical Chemistry B*, **2008**, 112, 242-9	3.4	81
72	Exploring atomistic details of pH-dependent peptide folding. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 18546-50	11.5	79
71	Bioinspired bio-voltage memristors. *Nature Communications*, **2020**, 11, 1861	17.4	79
70	Intrinsically disordered p53 extreme C-terminus binds to S100B(betabeta) through "fly-casting". *Journal of the American Chemical Society*, **2009**, 131, 2088-9	16.4	77
69	Residual structures, conformational fluctuations, and electrostatic interactions in the synergistic folding of two intrinsically disordered proteins. *PLoS Computational Biology*, **2012**, 8, e1002353	5	73
68	Towards the physical basis of how intrinsic disorder mediates protein function. *Archives of Biochemistry and Biophysics*, **2012**, 524, 123-31	4.1	67
67	Electrostatically accelerated encounter and folding for facile recognition of intrinsically disordered proteins. *PLoS Computational Biology*, **2013**, 9, e1003363	5	67
66	Application of torsion angle molecular dynamics for efficient sampling of protein conformations. *Journal of Computational Chemistry*, **2005**, 26, 1565-78	3.5	63
65	Electrostatically accelerated coupled binding and folding of intrinsically disordered proteins. *Journal of Molecular Biology*, **2012**, 422, 674-684	6.5	60
64	Topology-based modeling of intrinsically disordered proteins: balancing intrinsic folding and intermolecular interactions. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1251-66	4.2	60

63	Structural interpretation of paramagnetic relaxation enhancement-derived distances for disordered protein states. *Journal of Molecular Biology*, **2009**, 390, 467-77	6.5	60
62	Peptide and protein folding and conformational equilibria: theoretical treatment of electrostatics and hydrogen bonding with implicit solvent models. *Advances in Protein Chemistry*, **2005**, 72, 173-98		58
61	Model-free analysis of protein dynamics: assessment of accuracy and model selection protocols based on molecular dynamics simulation. *Journal of Biomolecular NMR*, **2004**, 29, 243-57	3	56
60	Refinement of NMR structures using implicit solvent and advanced sampling techniques. *Journal of the American Chemical Society*, **2004**, 126, 16038-47	16.4	53
59	Synergistic folding of two intrinsically disordered proteins: searching for conformational selection. *Molecular BioSystems*, **2012**, 8, 198-209		47
58	Atomistic modelling of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS). *Journal of Applied Crystallography*, **2016**, 49, 1861-1875	3.8	46
57	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	6.4	43
56	Intrinsically disordered proteins in a physics-based world. *International Journal of Molecular Sciences*, **2010**, 11, 5292-309	6.3	42
55	Molecular basis of PIP-dependent regulation of the Ca-activated chloride channel TMEM16A. *Nature Communications*, **2019**, 10, 3769	17.4	39
54	Critical importance of length-scale dependence in implicit modeling of hydrophobic interactions. *Journal of the American Chemical Society*, **2007**, 129, 2444-5	16.4	38
53	Hydrophobic gating in BK channels. *Nature Communications*, **2018**, 9, 3408	17.4	35
52	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	3	35
51	Accelerate Sampling in Atomistic Energy Landscapes Using Topology-Based Coarse-Grained Models. *Journal of Chemical Theory and Computation*, **2014**, 10, 918-23	6.4	32
50	FoldGPCR: structure prediction protocol for the transmembrane domain of G protein-coupled receptors from class A. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2189-201	4.2	31
49	Application of solid-state NMR restraint potentials in membrane protein modeling. *Journal of Magnetic Resonance*, **2008**, 193, 68-76	3	28
48	Modulation of the disordered conformational ensembles of the p53 transactivation domain by cancer-associated mutations. *PLoS Computational Biology*, **2015**, 11, e1004247	5	27
47	EGCG binds intrinsically disordered N-terminal domain of p53 and disrupts p53-MDM2 interaction. *Nature Communications*, **2021**, 12, 986	17.4	27
46	An inner activation gate controls TMEM16F phospholipid scrambling. *Nature Communications*, **2019**, 10, 1846	17.4	25

45	Multiscale filter diagonalization method for spectral analysis of noisy data with nonlocalized features. *Journal of Chemical Physics*, **2000**, 112, 4429-4437	3.9	25
44	Multiscale enhanced sampling of intrinsically disordered protein conformations. *Journal of Computational Chemistry*, **2016**, 37, 550-7	3.5	24
43	Efficiency of Adaptive Temperature-Based Replica Exchange for Sampling Large-Scale Protein Conformational Transitions. *Journal of Chemical Theory and Computation*, **2013**, 9, 2849-56	6.4	24
42	Potential conformational heterogeneity of p53 bound to S100B(*Journal of Molecular Biology*, **2013**, 425, 999-1010	6.5	22
41	Effective Approximation of Molecular Volume Using Atom-Centered Dielectric Functions in Generalized Born Models. *Journal of Chemical Theory and Computation*, **2010**, 6, 2790-803	6.4	22
40	Optimization of the GBMV2 implicit solvent force field for accurate simulation of protein conformational equilibria. *Journal of Computational Chemistry*, **2017**, 38, 1332-1341	3.5	21
39	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	11.5	21
38	Branched oligopeptides form nanocapsules with lipid vesicle characteristics. *Langmuir*, **2013**, 29, 14648-54	4	20
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	6.4	17
36	Force-induced unfolding simulations of the human Notch1 negative regulatory region: possible roles of the heterodimerization domain in mechanosensing. *PLoS ONE*, **2011**, 6, e22837	3.7	17
35	Modulation of Amyloid- 2 Conformation by Small Molecules Through Nonspecific Binding. *Journal of Chemical Theory and Computation*, **2019**, 15, 5169-5174	6.4	16
34	Targeting Intrinsically Disordered Proteins through Dynamic Interactions. *Biomolecules*, **2020**, 10,	5.9	16
33	Residual Structure Accelerates Binding of Intrinsically Disordered ACTR by Promoting Efficient Folding upon Encounter. *Journal of Molecular Biology*, **2019**, 431, 422-432	6.5	16
32	MEFA (multiepitope fusion antigen)-Novel Technology for Structural Vaccinology, Proof from Computational and Empirical Immunogenicity Characterization of an Enterotoxigenic (ETEC) Adhesin MEFA. *Journal of Vaccines & Vaccination*, **2017**, 8,		15
31	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	3.4	13
30	HyRes: a coarse-grained model for multi-scale enhanced sampling of disordered protein conformations. *Physical Chemistry Chemical Physics*, **2017**, 19, 32421-32432	3.6	13
29	Different Anomeric Sugar Bound States of Maltose Binding Protein Resolved by a Cytolysin A Nanopore Tweezer. *ACS Nano*, **2020**, 14, 1727-1737	16.7	12
28	Replica exchange with guided annealing for accelerated sampling of disordered protein conformations. *Journal of Computational Chemistry*, **2014**, 35, 1682-9	3.5	12

27	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	2.8	11
26	Specific PIP binding promotes calcium activation of TMEM16A chloride channels. *Communications Biology*, **2021**, 4, 259	6.7	10
25	Dynamics of the BH3-Only Protein Binding Interface of Bcl-xL. *Biophysical Journal*, **2015**, 109, 1049-57	2.9	9
24	Structural characterization of two pore-forming peptides: consequences of introducing a C-terminal tryptophan. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2238-50	4.2	7
23	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	3.5	7
22	The Levinthal Problem in Amyloid Aggregation: Sampling of a Flat Reaction Space. *Journal of Physical Chemistry B*, **2017**, 121, 1576-1586	3.4	6
21	Organization and Structure of Branched Amphipathic Oligopeptide Bilayers. *Langmuir*, **2016**, 32, 9883-94	4	6
20	Hydrophobic dewetting in gating and regulation of transmembrane protein ion channels. *Journal of Chemical Physics*, **2020**, 153, 110901	3.9	5
19	Necessity of high-resolution for coarse-grained modeling of flexible proteins. *Journal of Computational Chemistry*, **2016**, 37, 1725-33	3.5	5
18	Cancer-Associated Mutations Perturb the Disordered Ensemble and Interactions of the Intrinsically Disordered p53 Transactivation Domain. *Journal of Molecular Biology*, **2021**, 433, 167048	6.5	5
17	Effects of flanking loops on membrane insertion of transmembrane helices: a role for peptide conformational equilibrium. *Journal of Physical Chemistry B*, **2013**, 117, 8330-9	3.4	4
16	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	1.3	4
15	Atomistic Peptide Folding Simulations Reveal Interplay of Entropy and Long-Range Interactions in Folding Cooperativity. *Scientific Reports*, **2018**, 8, 13668	4.9	3
14	Advanced Sampling Methods for Multiscale Simulation of Disordered Proteins and Dynamic Interactions. *Biomolecules*, **2021**, 11,	5.9	3
13	Conformational Flexibility and pH Effects on Anisotropic Growth of Sheet-Like Assembly of Amphiphilic Peptides. *Journal of Nanoscience and Nanotechnology*, **2015**, 15, 4470-9	1.3	2
12	Accelerating atomistic simulations of proteins using multiscale enhanced sampling with independent tempering. *Journal of Computational Chemistry*, **2021**, 42, 358-364	3.5	2
11	Positional Isomers of a Non-Nucleoside Substrate Differentially Affect Myosin Function. *Biophysical Journal*, **2020**, 119, 567-580	2.9	1
10	Free energy analysis of conductivity and charge selectivity of M2GlyR-derived synthetic channels. *Biochimica Et Biophysica Acta - Biomembranes*, **2014**, 1838, 2319-25	3.8	1

9	Efficacy of independence sampling in replica exchange simulations of ordered and disordered proteins. *Journal of Computational Chemistry*, **2017**, 38, 2632-2640	3.5	1
8	Implicit Solvent Force-Field Optimization167-190		1
7	Computing Energy Levels by Inversion of Imaginary-Time Cross-Correlation Functions *Journal of Physical Chemistry A*, **2003**, 107, 7175-7180	2.8	1
6	Expression and Characterization of Stress Responsive Peptide-1; an Inducer of Antimicrobial Peptide Synthesis **2019**, 4, 42-52		1
5	Physics-based modeling provides predictive understanding of selectively promiscuous substrate binding by Hsp70 chaperones. *PLoS Computational Biology*, **2021**, 17, e1009567	5	1
4	Aromatic interactions with membrane modulate human BK channel activation. *ELife*, **2020**, 9,	8.9	1
3	Specific PIP2 Binding Promotes Calcium Activation of TMEM16A Chloride Channels		1
2	Intrinsically Disordered N-terminal Domain (NTD) of p53 Interacts with Mitochondrial PTP Regulator Cyclophilin D.. *Journal of Molecular Biology*, **2022**, 434, 167552	6.5	1
1	Atomistic Glimpse of the Orderly Chaos of One Protein. *Biophysical Journal*, **2015**, 109, 1511-2	2.9	