Jhih-Wei Chu

List of Publications by Year
in descending order

76	4,156	147801 31	114465 63
papers	citations	h-index	g-index

77	77	77	3830
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The multiscale coarse-graining method. I. A rigorous bridge between atomistic and coarse-grained models. Journal of Chemical Physics, 2008, 128, 244114.	3.0	651
2	The multiscale coarse-graining method. II. Numerical implementation for coarse-grained molecular models. Journal of Chemical Physics, 2008, 128, 244115.	3.0	326
3	Illuminating the mechanistic roles of enzyme conformational dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 18055-18060.	7.1	271
4	Multiscale Coarse-Graining and Structural Correlations:Â Connections to Liquid-State Theory. Journal of Physical Chemistry B, 2007, 111, 4116-4127.	2.6	191
5	Allostery of actin filaments: Molecular dynamics simulations and coarse-grained analysis. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13111-13116.	7.1	178
6	Coarse-Grained Modeling of the Actin Filament Derived from Atomistic-Scale Simulations. Biophysical Journal, 2006, 90, 1572-1582.	0.5	178
7	A super-linear minimization scheme for the nudged elastic band method. Journal of Chemical Physics, 2003, 119, 12708-12717.	3.0	163
8	On the Molecular Origins of Biomass Recalcitrance: The Interaction Network and Solvation Structures of Cellulose Microfibrils. Journal of Physical Chemistry B, 2010, 114, 13333-13341.	2.6	128
9	Coarse-Grained Free Energy Functions for Studying Protein Conformational Changes: A Double-Well Network Model. Biophysical Journal, 2007, 93, 3860-3871.	0.5	124
10	Dissecting Force Interactions in Cellulose Deconstruction Reveals the Required Solvent Versatility for Overcoming Biomass Recalcitrance. Journal of the American Chemical Society, 2011, 133, 14033-14041.	13.7	124
11	LWDâ€“TCP complex activates the morning gene CCA1 in Arabidopsis. Nature Communications, 2016, 7, 13181.	12.8	109
12	On the Mechanisms of Oxidation of Organic Sulfides by H2O2in Aqueous Solutions. Journal of the American Chemical Society, 2004, 126, 900-908.	13.7	98
13	Thermodynamics of Cellulose Solvation in Water and the Ionic Liquid 1-Butyl-3-Methylimidazolim Chloride. Journal of Physical Chemistry B, 2011, 115, 13433-13440.	2.6	86
14	Electrophoretic Mobility of a Sphere in a Spherical Cavity. Journal of Colloid and Interface Science, 1998, 205, 65-76.	9.4	85
15	The multiscale challenge for biomolecular systems: coarse-grained modeling. Molecular Simulation, 2006, 32, 211-218.	2.0	63
16	Emerging methods for multiscale simulation of biomolecular systems. Molecular Physics, 2007, 105, 167-175.	1.7	61
17	Intrinsic Bending and Structural Rearrangement of Tubulin Dimer: Molecular Dynamics Simulations and Coarse-Grained Analysis. Biophysical Journal, 2008, 95, 2487-2499.	0.5	61
18	Electrophoretic Mobility of a Concentrated Suspension of Spherical Particles. Journal of Colloid and Interface Science, 1999, 209, 240-246.	9.4	59

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19	Oxidation of Methionine Residues in Aqueous Solutions:â€‰ Free Methionine and Methionine in Granulocyte Colony-Stimulating Factor. Journal of the American Chemical Society, 2004, 126, 16601-16607.	13.7	56
20	A comprehensive picture of nonâ€site specific oxidation of methionine residues by peroxides in protein pharmaceuticals. Journal of Pharmaceutical Sciences, 2004, 93, 3096-3102.	3.3	54
21	Molecular Dynamics Simulations and Oxidation Rates of Methionine Residues of Granulocyte Colony-Stimulating Factor at Different pH Values. Biochemistry, 2004, 43, 1019-1029.	2.5	51
22	Bridging fluctuating hydrodynamics and molecular dynamics simulations of fluids. Journal of Chemical Physics, 2009, 130, 134111.	3.0	49
23	On the Roles of Substrate Binding and Hinge Unfolding in Conformational Changes of Adenylate Kinase. Biophysical Journal, 2010, 99, 3420-3429.	0.5	49
24	Electrophoretic Mobility of a Spherical Particle in a Spherical Cavity. Journal of Colloid and Interface Science, 1997, 196, 316-320.	9.4	46
25	Entropy of cellulose dissolution in water and in the ionic liquid 1-butyl-3-methylimidazolim chloride. Physical Chemistry Chemical Physics, 2012, 14, 8425.	2.8	46
26	Inversion of radial distribution functions to pair forces by solving the Yvonâ€“Bornâ€“Green equation iteratively. Journal of Chemical Physics, 2009, 131, 134107.	3.0	43
27	Effects of Antioxidants on the Hydrogen Peroxide-Mediated Oxidation of Methionine Residues in Granulocyte Colony-Stimulating Factor and Human Parathyroid Hormone Fragment 13-34. Pharmaceutical Research, 2004, 21, 2377-2383.	3.5	39
28	Systems-level Modeling with Molecular Resolution Elucidates the Rate-limiting Mechanisms of Cellulose Decomposition by Cellobiohydrolases. Journal of Biological Chemistry, 2013, 288, 29081-29089.	3.4	39
29	An incoherent feed-forward loop switches the Arabidopsis clock rapidly between two hysteretic states. Scientific Reports, 2018, 8, 13944.	3.3	36
30	APE1 distinguishes DNA substrates in exonucleolytic cleavage by induced space-filling. Nature Communications, 2021, 12, 601.	12.8	36
31	Effects of Excipients on the Hydrogen Peroxide-Induced Oxidation of Methionine Residues in Granulocyte Colony-Stimulating Factor. Pharmaceutical Research, 2005, 22, 141-147.	3.5	35
32	Fluctuating hydrodynamics for multiscale simulation of inhomogeneous fluids: Mapping all-atom molecular dynamics to capillary waves. Journal of Chemical Physics, 2011, 135, 044111.	3.0	35
33	Reaction Path Optimization with Holonomic Constraints and Kinetic Energy Potentials. Journal of Chemical Theory and Computation, 2009, 5, 2050-2061.	5.3	34
34	Importance of Internal Porosity for Glucan Adsorption in Mesoporous Carbon Materials. Langmuir, 2015, 31, 7288-7295.	3.5	30
35	Electrophoresis of a Sphere in a Spherical Cavity at Arbitrary Electrical Potentials. Langmuir, 2001, 17, 6289-6297.	3.5	29
36	Preferential Interactions between Lithium Chloride and Glucan Chains in N,N-Dimethylacetamide Drive Cellulose Dissolution. Journal of Physical Chemistry B, 2013, 117, 3280-3286.	2.6	29

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37	Expectation-Maximization of the Potential of Mean Force and Diffusion Coefficient in Langevin Dynamics from Single Molecule FRET Data Photon by Photon. Journal of Physical Chemistry B, 2013, 117, 15591-15605.	2.6	29
38	Structural basis for overhang excision and terminal unwinding of DNA duplexes by TREX1. PLoS Biology, 2018, 16, e2005653.	5.6	28
39	Sedimentation potential of a concentrated spherical colloidal suspension. Journal of Chemical Physics, 1999, 110, 11643-11651.	3.0	26
40	Deactivation of lipopolysaccharide by Ar and H₂inductively coupled low-pressure plasma. Journal Physics D: Applied Physics, 2014, 47, 045202.	2.8	26
41	A Structural and Mechanistic Study of the Oxidation of Methionine Residues in hPTH(1â^'34) via Experiments and Simulationsâ€. Biochemistry, 2004, 43, 14139-14148.	2.5	25
42	Plasma Deactivation of Endotoxic Biomolecules: Vacuum Ultraviolet Photon and Radical Beam Effects on Lipid A. Plasma Processes and Polymers, 2013, 10, 167-180.	3.0	25
43	Protein Allostery at the Solidâ€"Liquid Interface: Endoglucanase Attachment to Cellulose Affects Glucan Clenching in the Binding Cleft. Journal of the American Chemical Society, 2011, 133, 16617-16624.	13.7	22
44	Kinetic Modeling at Single-Molecule Resolution Elucidates the Mechanisms of Cellulase Synergy. ACS Catalysis, 2014, 4, 2216-2225.	11.2	20
45	Modeling the nanoscale viscoelasticity of fluids by bridging non-Markovian fluctuating hydrodynamics and molecular dynamics simulations. Journal of Chemical Physics, 2009, 131, 234115.	3.0	19
46	â€œFluctuogramsâ€•Reveal the Intermittent Intra-Protein Communication in Subtilisin Carlsberg and Correlate Mechanical Coupling with Co-Evolution. PLoS Computational Biology, 2011, 7, e1002023.	3.2	19
47	Atomistic and Coarse-grained Analysis of Double Spectrin Repeat Units: The Molecular Origins of Flexibility. Journal of Molecular Biology, 2007, 365, 523-534.	4.2	18
48	Decomposition of energy and free energy changes by following the flow of work along reaction path. Journal of Chemical Physics, 2009, 131, 144105.	3.0	18
49	Fluctuating hydrodynamics for multiscale modeling and simulation: Energy and heat transfer in molecular fluids. Journal of Chemical Physics, 2012, 137, 044117.	3.0	18
50	Trajectory Entropy of Continuous Stochastic Processes at Equilibrium. Journal of Physical Chemistry Letters, 2014, 5, 999-1003.	4.6	17
51	Analysis of Trajectory Entropy for Continuous Stochastic Processes at Equilibrium. Journal of Physical Chemistry B, 2014, 118, 8099-8107.	2.6	15
52	Structural distributions from single-molecule measurements as a tool for molecular mechanics. Chemical Physics, 2012, 396, 61-71.	1.9	14
53	Endoglucanase Peripheral Loops Facilitate Complexation of Glucan Chains on Cellulose via Adaptive Coupling to the Emergent Substrate Structures. Journal of Physical Chemistry B, 2013, 117, 10750-10758.	2.6	14
54	Confocal Single-Molecule FRET for Protein Conformational Dynamics. Methods in Molecular Biology, 2014, 1084, 51-62.	0.9	14

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55	Fisher information metric for the Langevin equation and least informative models of continuous stochastic dynamics. Journal of Chemical Physics, 2013, 139, 121931.	3.0	13
56	Degree of Polymerization of Glucan Chains Shapes the Structure Fluctuations and Melting Thermodynamics of a Cellulose Microfibril. Journal of Physical Chemistry B, 2012, 116, 8074-8083.	2.6	12
57	Understanding APE1 cellular functions by the structural preference of exonuclease activities. Computational and Structural Biotechnology Journal, 2021, 19, 3682-3691.	4.1	11
58	Modelling the viscoelasticity and thermal fluctuations of fluids at the nanoscale. Molecular Simulation, 2010, 36, 552-559.	2.0	10
59	Structure-mechanics statistical learning unravels the linkage between local rigidity and global flexibility in nucleic acids. Chemical Science, 2020, 11, 4969-4979.	7.4	10
60	Identifying the structural and kinetic elements in protein large-amplitude conformational motions. International Reviews in Physical Chemistry, 2017, 36, 185-227.	2.3	7
61	Sedimentation of Concentrated Charged Spheres at Low Surface Potentials. Langmuir, 2000, 16, 1650-1654.	3.5	5
62	Compound Molecular Logic in Accessing the Active Site of Mycobacterium tuberculosis Protein Tyrosine Phosphatase B. Journal of the American Chemical Society, 2018, 140, 14747-14752.	13.7	5
63	Mechanical couplings of protein backbone and side chains exhibit scale-free network properties and specific hotspots for function. Computational and Structural Biotechnology Journal, 2021, 19, 5309-5320.	4.1	5
64	Linking hydrophobicity and hydrodynamics by the hybrid fluctuating hydrodynamics and molecular dynamics methodologies. Physical Review E, 2013, 88, 023305.	2.1	4
65	Structure-mechanics statistical learning uncovers mechanical relay in proteins. Chemical Science, 2022, 13, 3688-3696.	7.4	4
66	Basal leakage in oscillation: Coupled transcriptional and translational control using feed-forward loops. PLoS Computational Biology, 2020, 16, e1007740.	3.2	3
67	Targeted Covalent Inhibitors Allosterically Deactivate the DEDDh Lassa Fever Virus NP Exonuclease from Alternative Distal Sites. Jacs Au, 2021, 1, 2315-2327.	7.9	3
68	Calculation of Enzyme Fluctuograms from All-Atom Molecular Dynamics Simulation. Methods in Enzymology, 2016, 578, 327-342.	1.0	2
69	Edge weights in a protein elastic network reorganize collective motions and render long-range sensitivity responses. Journal of Chemical Physics, 2022, 156, .	3.0	2
70	Dynamic mesoscale model of dipolar fluids via fluctuating hydrodynamics. Journal of Chemical Physics, 2014, 141, 174105.	3.0	1
71	On the Development of State-Specific Coarse-Grained Potentials of Water. , 0, , 233-250.		0
72	Thermodynamics of cellulose solvation in novel solvent mixtures. FASEB Journal, 2013, 27, .	0.5	0

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73	Title is missing!. , 2020, 16, e1007740.		0
74	Title is missing!. , 2020, 16, e1007740.		0
75	Title is missing!. , 2020, 16, e1007740.		0
76	Title is missing!. , 2020, 16, e1007740.		0