

Xiaolin Cheng

List of Publications by Year in descending order

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109
papers

3,320
citations

147801

31
h-index

182427

51
g-index

112
all docs

112
docs citations

112
times ranked

4573
citing authors

#	ARTICLE	IF	CITATIONS
1	Enantioselective Electrophilic Trifluoromethylthiolation of α -Ketoesters: A Case of Reactivity and Selectivity Bias for Organocatalysis. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 12860-12864.	13.8	203
2	The dynamics of single protein molecules is non-equilibrium and self-similar over thirteen decades in time. <i>Nature Physics</i> , 2016, 12, 171-174.	16.7	140
3	The in vivo structure of biological membranes and evidence for lipid domains. <i>PLoS Biology</i> , 2017, 15, e2002214.	5.6	123
4	Cosolvent pretreatment in cellulosic biofuel production: effect of tetrahydrofuran-water on lignin structure and dynamics. <i>Green Chemistry</i> , 2016, 18, 1268-1277.	9.0	122
5	Biological Membrane Organization and Cellular Signaling. <i>Chemical Reviews</i> , 2019, 119, 5849-5880.	47.7	112
6	Mechanical Properties of Nanoscopic Lipid Domains. <i>Journal of the American Chemical Society</i> , 2015, 137, 15772-15780.	13.7	108
7	Lateral organization, bilayer asymmetry, and inter-leaflet coupling of biological membranes. <i>Chemistry and Physics of Lipids</i> , 2015, 192, 87-99.	3.2	104
8	Local Phase Separation of Co-solvents Enhances Pretreatment of Biomass for Bioenergy Applications. <i>Journal of the American Chemical Society</i> , 2016, 138, 10869-10878.	13.7	89
9	Generation of the configurational ensemble of an intrinsically disordered protein from unbiased molecular dynamics simulation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 20446-20452.	7.1	88
10	The molecular structure of a phosphatidylserine bilayer determined by scattering and molecular dynamics simulations. <i>Soft Matter</i> , 2014, 10, 3716.	2.7	84
11	A new crystal form of human acetylcholinesterase for exploratory room-temperature crystallography studies. <i>Chemico-Biological Interactions</i> , 2019, 309, 108698.	4.0	82
12	A Multifunctional Cosolvent Pair Reveals Molecular Principles of Biomass Deconstruction. <i>Journal of the American Chemical Society</i> , 2019, 141, 12545-12557.	13.7	73
13	The Role of Histone Tails in the Nucleosome: A Computational Study. <i>Biophysical Journal</i> , 2014, 107, 2911-2922.	0.5	70
14	Description of Hydration Water in Protein (Green Fluorescent Protein) Solution. <i>Journal of the American Chemical Society</i> , 2017, 139, 1098-1105.	13.7	68
15	Structural and mechanical properties of cardiolipin lipid bilayers determined using neutron spin echo, small angle neutron and X-ray scattering, and molecular dynamics simulations. <i>Soft Matter</i> , 2015, 11, 130-138.	2.7	65
16	Heterohexamers Formed by CcmK3 and CcmK4 Increase the Complexity of Beta Carboxysome Shells. <i>Plant Physiology</i> , 2019, 179, 156-167.	4.8	61
17	Simulation of a cellulose fiber in ionic liquid suggests a synergistic approach to dissolution. <i>Cellulose</i> , 2014, 21, 983-997.	4.9	58
18	Interactions of the Anticancer Drug Tamoxifen with Lipid Membranes. <i>Biophysical Journal</i> , 2015, 108, 2492-2501.	0.5	55

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19	An Explicit, Multi-Factor Credit Default Swap Pricing Model with Correlated Factors. <i>Journal of Financial and Quantitative Analysis</i> , 2008, 43, 123-160.	3.5	53
20	A Solvent-Free Coarse Grain Model for Crystalline and Amorphous Cellulose Fibrils. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2539-2548.	5.3	52
21	Neutron scattering in the biological sciences: progress and prospects. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 1129-1168.	2.3	47
22	Surface Hydration Amplifies Single-Well Protein Atom Diffusion Propagating into the Macromolecular Core. <i>Physical Review Letters</i> , 2012, 108, 238102.	7.8	45
23	Temperature-Dependent Lipid Extraction from Membranes by Boron Nitride Nanosheets. <i>ACS Nano</i> , 2018, 12, 2764-2772.	14.6	44
24	AFMPB: An adaptive fast multipole Poisson-Boltzmann solver for calculating electrostatics in biomolecular systems. <i>Computer Physics Communications</i> , 2010, 181, 1150-1160.	7.5	42
25	<i>Bacillus subtilis</i> Lipid Extract, A Branched-Chain Fatty Acid Model Membrane. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4214-4217.	4.6	42
26	Lipid Rafts: Buffers of Cell Membrane Physical Properties. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2050-2056.	2.6	40
27	Temperature-dependent phase behaviour of tetrahydrofuran-water alters solubilization of xylan to improve co-production of furfurals from lignocellulosic biomass. <i>Green Chemistry</i> , 2018, 20, 1612-1620.	9.0	39
28	Molecular-Dynamics Simulations of ELIC, a Prokaryotic Homologue of the Nicotinic Acetylcholine Receptor. <i>Biophysical Journal</i> , 2009, 96, 4502-4513.	0.5	36
29	Interactions between Ether Phospholipids and Cholesterol As Determined by Scattering and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14829-14838.	2.6	36
30	Molecular Dynamics. <i>Methods in Molecular Biology</i> , 2012, 929, 243-285.	0.9	36
31	Synthesis, docking, and biological studies of phenanthrene \hat{I}^2 -diketo acids as novel HIV-1 integrase inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 6146-6151.	2.2	35
32	<i>Listeria monocytogenes</i> upregulates mitochondrial calcium signalling to inhibit LC3-associated phagocytosis as a survival strategy. <i>Nature Microbiology</i> , 2021, 6, 366-379.	13.3	33
33	Preclinical Validation of the Heparin-Reactive Peptide p5+14 as a Molecular Imaging Agent for Visceral Amyloidosis. <i>Molecules</i> , 2015, 20, 7657-7682.	3.8	30
34	Determination of functional collective motions in a protein at atomic resolution using coherent neutron scattering. <i>Science Advances</i> , 2016, 2, e1600886.	10.3	30
35	Molecular Driving Forces behind the Tetrahydrofuran-Water Miscibility Gap. <i>Journal of Physical Chemistry B</i> , 2016, 120, 740-747.	2.6	30
36	Replica-Exchange Molecular Dynamics Simulations of Cellulose Solvated in Water and in the Ionic Liquid 1-Butyl-3-Methylimidazolium Chloride. <i>Journal of Physical Chemistry B</i> , 2014, 118, 11037-11049.	2.6	29

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37	Organosolv-Water Cosolvent Phase Separation on Cellulose and its Influence on the Physical Deconstruction of Cellulose: A Molecular Dynamics Analysis. <i>Scientific Reports</i> , 2017, 7, 14494.	3.3	29
38	STarFish: A Stacked Ensemble Target Fishing Approach and its Application to Natural Products. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4906-4920.	5.4	27
39	Branched-Chain Fatty Acid Content Modulates Structure, Fluidity, and Phase in Model Microbial Cell Membranes. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5814-5821.	2.6	27
40	Molecular Dynamics Investigation of the Substrate Binding Mechanism in Carboxylesterase. <i>Biochemistry</i> , 2015, 54, 1841-1848.	2.5	25
41	Enhanced sampling simulation analysis of the structure of lignin in the THF-water miscibility gap. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6394-6398.	2.8	24
42	Carotenoids promote lateral packing and condensation of lipid membranes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12281-12293.	2.8	24
43	Rational design, synthesis, and evaluation of uncharged, <i>smart</i> -bis-oxime antidotes of organophosphate-inhibited human acetylcholinesterase. <i>Journal of Biological Chemistry</i> , 2020, 295, 4079-4092.	3.4	24
44	Analysis of the solution structure of <i>Thermosynechococcus elongatus</i> photosystem I in n-dodecyl- β -D-maltoside using small-angle neutron scattering and molecular dynamics simulation. <i>Archives of Biochemistry and Biophysics</i> , 2014, 550-551, 50-57.	3.0	23
45	Na ⁺ /K ⁺ -ATPase-Targeted Cytotoxicity of (+)-Digoxin and Several Semisynthetic Derivatives. <i>Journal of Natural Products</i> , 2020, 83, 638-648.	3.0	23
46	Ab Initio Study of Molecular Interactions in Cellulose I β . <i>Journal of Physical Chemistry B</i> , 2013, 117, 10430-10443.	2.6	22
47	Coarse-Grain Model for Natural Cellulose Fibrils in Explicit Water. <i>Journal of Physical Chemistry B</i> , 2014, 118, 3026-3034.	2.6	22
48	Probing the structural requirements of polybasic peptides for effective and specific amyloid reactivity. <i>Amyloid: the International Journal of Experimental and Clinical Investigation: the Official Journal of the International Society of Amyloidosis</i> , 2017, 24, 30-31.	3.0	22
49	Structural relaxation, viscosity, and network connectivity in a hydrogen bonding liquid. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25859-25869.	2.8	22
50	Ordering of lipid membranes altered by boron nitride nanosheets. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3903-3910.	2.8	22
51	The structures of polyunsaturated lipid bilayers by joint refinement of neutron and X-ray scattering data. <i>Chemistry and Physics of Lipids</i> , 2020, 229, 104892.	3.2	21
52	Improved Conformational Sampling through an Efficient Combination of Mean-Field Simulation Approaches. <i>Journal of Physical Chemistry B</i> , 2004, 108, 426-437.	2.6	20
53	Structure and Dynamics of a Compact State of a Multidomain Protein, the Mercuric Ion Reductase. <i>Biophysical Journal</i> , 2014, 107, 393-400.	0.5	19
54	Simulation analysis of the cellulase Cel7A carbohydrate binding module on the surface of the cellulose I β . <i>Cellulose</i> , 2014, 21, 951-971.	4.9	19

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55	Behavior of Bilayer Leaflets in Asymmetric Model Membranes: Atomistic Simulation Studies. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8438-8448.	2.6	19
56	Theoretical Study of the Initial Stages of Self-Assembly of a Carboxysome's Facet. <i>ACS Nano</i> , 2016, 10, 5751-5758.	14.6	19
57	Effects of carotenoids on lipid bilayers. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3795-3804.	2.8	19
58	Limitations in current acetylcholinesterase structure-based design of oxime antidotes for organophosphate poisoning. <i>Annals of the New York Academy of Sciences</i> , 2016, 1378, 41-49.	3.8	17
59	Insecticidal and Antifeedant Activities of Malagasy Medicinal Plant (<i>Cinnamosma</i> sp.) Extracts and Drimane-Type Sesquiterpenes against <i>Aedes aegypti</i> Mosquitoes. <i>Insects</i> , 2019, 10, 373.	2.2	17
60	Controlling the Revolving and Rotating Motion Direction of Asymmetric Hexameric Nanomotor by Arginine Finger and Channel Chirality. <i>ACS Nano</i> , 2019, 13, 6207-6223.	14.6	17
61	Computational and Experimental Approaches to Investigate Lipid Nanoparticles as Drug and Gene Delivery Systems. <i>Current Topics in Medicinal Chemistry</i> , 2021, 21, 92-114.	2.1	16
62	Quasielastic neutron scattering in biology: Theory and applications. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017, 1861, 3638-3650.	2.4	15
63	Modeling of the Passive Permeation of Mercury and Methylmercury Complexes Through a Bacterial Cytoplasmic Membrane. <i>Environmental Science & Technology</i> , 2017, 51, 10595-10604.	10.0	15
64	Impact of Resistance Mutations on Inhibitor Binding to HIV-1 Integrase. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 3297-3307.	5.4	14
65	Cytotoxic and non-cytotoxic cardiac glycosides isolated from the combined flowers, leaves, and twigs of <i>Streblus asper</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115301.	3.0	14
66	All-Atom Molecular Dynamics Simulation of a Photosystem I/Detergent Complex. <i>Journal of Physical Chemistry B</i> , 2014, 118, 11633-11645.	2.6	13
67	Productive reorientation of a bound oxime reactivator revealed in room temperature X-ray structures of native and VX-inhibited human acetylcholinesterase. <i>Journal of Biological Chemistry</i> , 2019, 294, 10607-10618.	3.4	13
68	Mathematical and Numerical Aspects of the Adaptive Fast Multipole Poisson-Boltzmann Solver. <i>Communications in Computational Physics</i> , 2013, 13, 107-128.	1.7	12
69	Morphology-Induced Defects Enhance Lipid Transfer Rates. <i>Langmuir</i> , 2016, 32, 9757-9764.	3.5	11
70	Comparative exploration of hydrogen sulfide and water transmembrane free energy surfaces via orthogonal space tempering free energy sampling. <i>Journal of Computational Chemistry</i> , 2016, 37, 567-574.	3.3	11
71	Structurally Modified Cyclopenta[<i>b</i>]benzofuran Analogues Isolated from <i>Aglaia perviridis</i> . <i>Journal of Natural Products</i> , 2019, 82, 2870-2877.	3.0	11
72	SCNrank: spectral clustering for network-based ranking to reveal potential drug targets and its application in pancreatic ductal adenocarcinoma. <i>BMC Medical Genomics</i> , 2020, 13, 50.	1.5	11

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73	Facilitative lysosomal transport of bile acids alleviates ER stress in mouse hematopoietic precursors. <i>Nature Communications</i> , 2021, 12, 1248.	12.8	11
74	Structure and Function of Photosystem I [FeFe] Hydrogenase Protein Fusions: An All-Atom Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2016, 120, 599-609.	2.6	10
75	Molecular dynamics simulation studies of the wild type and E92Q/N155H mutant of Elvitegravir-resistance HIV-1 integrase. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2015, 7, 36-42.	3.6	9
76	Secondary structure propensity and chirality of the amyloidophilic peptide p5 and its analogues impacts ligand binding - In vitro characterization. <i>Biochemistry and Biophysics Reports</i> , 2016, 8, 89-99.	1.3	9
77	Rational Design of Small Molecules to Enhance Genome Editing Efficiency by Selectively Targeting Distinct Functional States of CRISPR-Cas12a. <i>Bioconjugate Chemistry</i> , 2020, 31, 542-546.	3.6	9
78	Structural Insights into the Interactions of Digoxin and Na ⁺ /K ⁺ -ATPase and Other Targets for the Inhibition of Cancer Cell Proliferation. <i>Molecules</i> , 2021, 26, 3672.	3.8	9
79	Development of Murine Leukemia Virus Integrase-Derived Peptides That Bind Brd4 Extra-Terminal Domain as Candidates for Suppression of Acute Myeloid Leukemia. <i>ACS Pharmacology and Translational Science</i> , 2021, 4, 1628-1638.	4.9	9
80	In Vitro and In Vivo Inhibition of MATE1 by Tyrosine Kinase Inhibitors. <i>Pharmaceutics</i> , 2021, 13, 2004.	4.5	9
81	Rational design of a carboxylic esterase RhEst1 based on computational analysis of substrate binding. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 62, 319-324.	2.4	8
82	The tilt-dependent potential of mean force of a pair of DNA oligomers from all-atom molecular dynamics simulations. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 084002.	1.8	8
83	Computationally Guided Discovery and Experimental Validation of Indole-3-acetic Acid Synthesis Pathways. <i>ACS Chemical Biology</i> , 2019, 14, 2867-2875.	3.4	8
84	Activated nanoscale actin-binding domain motion in the catenin-cadherin complex revealed by neutron spin echo spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	8
85	Covalent inhibition of hAChE by organophosphates causes homodimer dissociation through long-range allosteric effects. <i>Journal of Biological Chemistry</i> , 2021, 297, 101007.	3.4	8
86	Structural Insights into gp16 ATPase in the Bacteriophage ϕ 29 DNA Packaging Motor. <i>Biochemistry</i> , 2021, 60, 886-897.	2.5	7
87	Relative Binding Affinities of Monolignols to Horseradish Peroxidase. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7635-7640.	2.6	6
88	Synthesis and biological evaluation of aminothiazoles against <i>Histoplasma capsulatum</i> and <i>Cryptococcus neoformans</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2018, 26, 2251-2261.	3.0	6
89	Structural investigation of the enantioselectivity and thermostability mechanisms of esterase RhEst1. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 85, 182-189.	2.4	6
90	Lipid extraction by boron nitride nanosheets from liquid-ordered and liquid-disordered nanodomains. <i>Nanoscale</i> , 2018, 10, 14073-14081.	5.6	6

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91	Semi-synthetic cinnamodial analogues: Structural insights into the insecticidal and antifeedant activities of drimane sesquiterpenes against the mosquito <i>Aedes aegypti</i> . <i>PLoS Neglected Tropical Diseases</i> , 2020, 14, e0008073.	3.0	6
92	Interaction of (+)-Strebloside and Its Derivatives with Na ⁺ /K ⁺ -ATPase and Other Targets. <i>Molecules</i> , 2021, 26, 5675.	3.8	6
93	AFMPB: An adaptive fast multipole Poisson-Boltzmann solver for calculating electrostatics in biomolecular systems. <i>Computer Physics Communications</i> , 2013, 184, 2618-2619.	7.5	5
94	Atomistic Simulation of Lignocellulosic Biomass and Associated Cellulosomal Protein Complexes. <i>ACS Symposium Series</i> , 2010, , 55-73.	0.5	4
95	Mechanistic Insights into the Allosteric Inhibition of Androgen Receptors by Binding Function 3 Antagonists from an Integrated Molecular Modeling Study. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3477-3494.	5.4	4
96	Generalized Ensemble Sampling of Enzyme Reaction Free Energy Pathways. <i>Methods in Enzymology</i> , 2016, 577, 57-74.	1.0	3
97	Reply to: Insufficient evidence for ageing in protein dynamics. <i>Nature Physics</i> , 2021, 17, 775-776.	16.7	3
98	Computational investigation of the binding of a designed peptide to β light chain amyloid fibril. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20634-20644.	2.8	2
99	Description of Hydration Water in Protein (GFP) Solution. <i>Biophysical Journal</i> , 2017, 112, 201a.	0.5	1
100	21. Molecular dynamics simulation studies of small molecules interacting with cell membranes. , 2019, , 603-630.		1
101	Direct structural evidence supporting a revolving mechanism in DNA packaging motors. <i>Biophysics Reports</i> , 2020, 6, 155-158.	0.8	1
102	A computational study of effects on membrane recruitment of the polar linkers in Vitamin E derivatives. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020, 1864, 129655.	2.4	1
103	Serendipitous inhibition of A β 2 and rV β 6W β amyloid fibril growth by bi-functional peptides. <i>Amyloid: the International Journal of Experimental and Clinical Investigation: the Official Journal of the International Society of Amyloidosis</i> , 2017, 24, 32-33.	3.0	0
104	The Effect of Organophosphate (OP)-Induced Structural Changes in Acetylcholinesterase on Kinetics of OP Inhibition and Oxime Reactivation. <i>FASEB Journal</i> , 2018, 32, 526.40.	0.5	0
105	Dynamics of Organophosphate-Induced Structural Changes in Acetylcholinesterase Revealed by Time-Resolved Small-Angle X-Ray Scattering and Inelastic Neutron Scattering. <i>FASEB Journal</i> , 2018, 32, 527.7.	0.5	0
106	Crystallographic studies of human acetylcholinesterase inhibition by organophosphates and reactivation by oximes. <i>FASEB Journal</i> , 2018, 32, 527.10.	0.5	0
107	Abstract 4257: Integrated network analysis reveals potentially novel molecular pathways mechanism and therapeutic targets of pancreatic ductal adenocarcinoma. , 2019, , .		0
108	Lines of communication within and between catalytic subunits of human acetylcholinesterase revealed by cryo- and room-temperature X-ray crystallography and by Small Angle X-ray Scattering (SAXS). , 0, , .		0

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109	Accelerating structure-based design of rapid uncharged reactivators of organophosphate-inhibited human acetylcholinesterase by joint X-ray/neutron mechanistic studies. , 0, , .		0