Jian Zhou

List of Publications by Citations

130 papers	4,309 citations	37 h-index	59 g-index
136 ext. papers	4,960 ext. citations	4.6 avg, IF	5.92 L-index

#	Paper	IF	Citations
130	Controlling Antibody Orientation on Charged Self-Assembled Monolayers. *Langmuir*, **2003**, 19, 2859-2864	4	209
129	Coarse-grained peptide modeling using a systematic multiscale approach. *Biophysical Journal*, **2007**, 92, 4289-303	2.9	160
128	Bioinspired graphene nanopores with voltage-tunable ion selectivity for Na(+) and K(+). *ACS Nano*, **2013**, 7, 10148-57	16.7	153
127	Molecular Simulation Studies of the Orientation and Conformation of Cytochrome c Adsorbed on Self-Assembled Monolayers. *Journal of Physical Chemistry B*, **2004**, 108, 17418-17424	3.4	132
126	Diameter and helicity effects on static properties of water molecules confined in carbon nanotubes. *Physical Chemistry Chemical Physics*, **2004**, 6, 829	3.6	131
125	Molecular dynamics study on ionic hydration. *Fluid Phase Equilibria*, **2002**, 194-197, 257-270	2.5	129
124	An ethane-trapping MOF PCN-250 for highly selective adsorption of ethane over ethylene. *Chemical Engineering Science*, **2018**, 175, 110-117	4.4	125
123	Orientation of Adsorbed Antibodies on Charged Surfaces by Computer Simulation Based on a United-Residue Model. *Langmuir*, **2003**, 19, 3472-3478	4	116
122	Anomalous hydration shell order of Na+ and K+ inside carbon nanotubes. *Nano Letters*, **2009**, 9, 989-94	11.5	99
121	Monte Carlo simulations of antibody adsorption and orientation on charged surfaces. *Journal of Chemical Physics*, **2004**, 121, 1050-7	3.9	84
120	Polydopamine-based synthesis of a zeolite imidazolate framework ZIF-100 membrane with high H2/CO2 selectivity. *Journal of Materials Chemistry A*, **2015**, 3, 4722-4728	13	82
119	Noble Gas Adsorption in Copper Trimesate, HKUST-1: An Experimental and Computational Study. *Journal of Physical Chemistry C*, **2013**, 117, 20116-20126	3.8	80
118	Peptide folding using multiscale coarse-grained models. *Journal of Physical Chemistry B*, **2008**, 112, 13079-90	3.4	79
117	Parallel tempering Monte Carlo simulations of lysozyme orientation on charged surfaces. *Journal of Chemical Physics*, **2010**, 132, 065101	3.9	70
116	Molecular simulation study of temperature effect on ionic hydration in carbon nanotubes. *Physical Chemistry Chemical Physics*, **2008**, 10, 1896-906	3.6	70
115	High-throughput computational screening of 137953 metal–organic frameworks for membrane separation of a CO2/N2/CH4 mixture. *Journal of Materials Chemistry A*, **2016**, 4, 15904-15912	13	70
114	Probing carbon nanotube–amino acid interactions in aqueous solution with molecular dynamics simulations. *Carbon*, **2014**, 78, 500-509	10.4	66

113	Prediction of diffusion coefficients for gas, liquid and supercritical fluid: application to pure real fluids and infinite dilute binary solutions based on the simulation of Lennard□ones fluid. *Fluid Phase Equilibria*, **2002**, 194-197, 1141-1159	2.5	65
112	Phase Behavior of Mixed Self-Assembled Monolayers of Alkanethiols on Au(111):□A Configurational-Bias Monte Carlo Simulation Study. *Langmuir*, **2001**, 17, 7566-7572	4	63
111	Design of amine-functionalized metal-organic frameworks for CO2 separation: the more amine, the better?. *Chemical Communications*, **2016**, 52, 974-7	5.8	62
110	Lipase adsorption on different nanomaterials: a multi-scale simulation study. *Physical Chemistry Chemical Physics*, **2015**, 17, 840-50	3.6	60
109	Ferroelectric ordering in ice nanotubes confined in carbon nanotubes. *Nano Letters*, **2008**, 8, 2607-12	11.5	60
108	Effect of composition on the formation of poly(dl-lactide) microspheres for drug delivery systems: Mesoscale simulations. *Chemical Engineering Journal*, **2007**, 131, 195-201	14.7	60
107	Adsorption of hydrophobin on different self-assembled monolayers: the role of the hydrophobic dipole and the electric dipole. *Langmuir*, **2014**, 30, 11401-11	4	56
106	Diffusion of water molecules confined in slits of rutile TiO2(1 1 0) and graphite(0 0 0 1). *Fluid Phase Equilibria*, **2011**, 302, 316-320	2.5	54
105	Adsorption and Diffusion of Supercritical Carbon Dioxide in Slit Pores. *Langmuir*, **2000**, 16, 8063-8070	4	53
104	Mesoscopic coarse-grained simulations of lysozyme adsorption. *Journal of Physical Chemistry B*, **2014**, 118, 4451-60	3.4	52
103	Ice-like Water Structure in Carbon Nanotube (8,8) Induces Cationic Hydration Enhancement. *Journal of Physical Chemistry C*, **2013**, 117, 11412-11420	3.8	49
102	Multiscale simulations of protein G B1 adsorbed on charged self-assembled monolayers. *Langmuir*, **2013**, 29, 11366-74	4	47
101	Effects of external electric fields on lysozyme adsorption by molecular dynamics simulations. *Biophysical Chemistry*, **2013**, 179, 26-34	3.5	46
100	Molecular Dynamics Study on Diameter Effect in Structure of Ethanol Molecules Confined in Single-Walled Carbon Nanotubes□ *Journal of Physical Chemistry C*, **2007**, 111, 15677-15685	3.8	46
99	Computer simulations of fibronectin adsorption on hydroxyapatite surfaces. *RSC Advances*, **2014**, 4, 15759	3.7	41
98	Understanding the curvature effect of silica nanoparticles on lysozyme adsorption orientation and conformation: a mesoscopic coarse-grained simulation study. *Physical Chemistry Chemical Physics*, **2016**, 18, 23500-7	3.6	40
97	Molecular simulations on nanoconfined water molecule behaviors for nanoporous material applications. *Microfluidics and Nanofluidics*, **2013**, 15, 191-205	2.8	39
96	Molecular Understanding of the Penetration of Functionalized Gold Nanoparticles into Asymmetric Membranes. *Langmuir*, **2017**, 33, 361-371	4	38

95	Molecular dynamics simulations of peptide adsorption on self-assembled monolayers. *Applied Surface Science*, **2012**, 258, 8153-8159	6.7	38
94	Computer simulations on the pH-sensitive tri-block copolymer containing zwitterionic sulfobetaine as a novel anti-cancer drug carrier. *Colloids and Surfaces B: Biointerfaces*, **2017**, 152, 260-268	6	37
93	Replica-exchange molecular dynamics simulation of basic fibroblast growth factor adsorption on hydroxyapatite. *Journal of Physical Chemistry B*, **2014**, 118, 5843-52	3.4	37
92	Effect of water content on microstructures and oxygen permeation in PSiMAIPNPMPC hydrogel: a molecular simulation study. *Chemical Engineering Science*, **2012**, 78, 236-245	4.4	37
91	Selective Adsorption of Light Alkanes on a Highly Robust Indium Based MetalOrganic Framework. *Industrial & Engineering Chemistry Research*, **2017**, 56, 4488-4495	3.9	36
90	Ribonuclease A adsorption onto charged self-assembled monolayers: A multiscale simulation study. *Chemical Engineering Science*, **2015**, 121, 331-339	4.4	34
89	Influence of hydrogen bonds and double bonds on the alkane and alkene derivatives self-assembled monolayers on HOPG surface: STM observation and computer simulation. *Applied Surface Science*, **2010**, 256, 4647-4655	6.7	34
88	Molecular dynamics simulations of conformation changes of HIV-1 regulatory protein on graphene. *Applied Surface Science*, **2016**, 377, 324-334	6.7	34
87	Molecular dynamics investigation on the infinite dilute diffusion coefficients of organic compounds in supercritical carbon dioxide. *Fluid Phase Equilibria*, **2000**, 172, 279-291	2.5	33
86	Unusual Moisture-Enhanced CO Capture within Microporous PCN-250 Frameworks. *ACS Applied Materials & Interfaces*, **2018**, 10, 38638-38647	9.5	33
85	Protein Translocation through a MoS2 Nanopore:A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2018**, 122, 2070-2080	3.8	32
84	Self-assembled core-shell and Janus microphase separated structures of polymer blends in aqueous solution. *Journal of Chemical Physics*, **2013**, 139, 084907	3.9	32
83	Molecular Understanding on the Underwater Oleophobicity of Self-Assembled Monolayers: Zwitterionic versus Nonionic. *Langmuir*, **2017**, 33, 1732-1741	4	31
82	Molecular dynamics simulations on the melting of gold nanoparticles. *Phase Transitions*, **2014**, 87, 59-70	1.3	30
81	Solvent-Responsive Behavior of Polymer-Brush-Modified Amphiphilic Gold Nanoparticles. *Macromolecular Theory and Simulations*, **2013**, 22, 174-186	1.5	30
80	Multiscale modeling and simulations of protein adsorption: progresses and perspectives. *Current Opinion in Colloid and Interface Science*, **2019**, 41, 74-85	7.6	30
79	Mesoscopic coarse-grained simulations of hydrophobic charge induction chromatography (HCIC) for protein purification. *AICHE Journal*, **2015**, 61, 2035-2047	3.6	28
78	Magnetic ZIF-8/cellulose/Fe3O4 nanocomposite: preparation, characterization, and enzyme immobilization. *Bioresources and Bioprocessing*, **2017**, 4,	5.2	27

77	Highly Efficient Enzymatic Acylation of Dihydromyricetin by the Immobilized Lipase with Deep Eutectic Solvents as Cosolvent. *Journal of Agricultural and Food Chemistry*, **2017**, 65, 2084-2088	5.7	26
76	Simulation insight into the cytochrome c adsorption on graphene and graphene oxide surfaces. *Applied Surface Science*, **2018**, 428, 825-834	6.7	25
75	Interfacial and phase transfer behaviors of polymer brush grafted amphiphilic nanoparticles: a computer simulation study. *Langmuir*, **2014**, 30, 5599-608	4	25
74	Unbinding of the streptavidin-biotin complex by atomic force microscopy: a hybrid simulation study. *Journal of Chemical Physics*, **2006**, 125, 104905	3.9	25
73	Electrostatics-mediated □-chymotrypsin inhibition by functionalized single-walled carbon nanotubes. *Physical Chemistry Chemical Physics*, **2017**, 19, 986-995	3.6	24
72	Molecular Simulations of Cytochrome c Adsorption on a Bare Gold Surface: Insights for the Hindrance of Electron Transfer. *Journal of Physical Chemistry C*, **2015**, 119, 20773-20781	3.8	23
71	Ionic Liquid Confined in Nafion: Toward Molecular-Level Understanding. *AICHE Journal*, **2013**, 59, 2630-2639	3.6	23
70	Molecular simulations of cytochrome c adsorption on positively charged surfaces: the influence of anion type and concentration. *Physical Chemistry Chemical Physics*, **2016**, 18, 9979-89	3.6	22
69	Lysozyme orientation and conformation on MoS surface: Insights from molecular simulations. *Biointerphases*, **2017**, 12, 02D416	1.8	22
68	Structural properties of polymer-brush-grafted gold nanoparticles at the oil-water interface: insights from coarse-grained simulations. *Soft Matter*, **2016**, 12, 3352-9	3.6	21
67	Structures and properties of PAMAM dendrimer: A multi-scale simulation study. *Fluid Phase Equilibria*, **2011**, 302, 43-47	2.5	21
66	Bilirubin Oxidase Adsorption onto Charged Self-Assembled Monolayers: Insights from Multiscale Simulations. *Langmuir*, **2018**, 34, 9818-9828	4	20
65	Molecular Understanding of Laccase Adsorption on Charged Self-Assembled Monolayers. *Journal of Physical Chemistry B*, **2017**, 121, 10610-10617	3.4	20
64	Understanding the Cellular Uptake of pH-Responsive Zwitterionic Gold Nanoparticles: A Computer Simulation Study. *Langmuir*, **2017**, 33, 14480-14489	4	20
63	A mechanical nanogate based on a carbon nanotube for reversible control of ion conduction. *Nanoscale*, **2014**, 6, 3686-94	7.7	19
62	Molecular simulation on the separation of water/ethanol azeotropic mixture by poly(vinyl alcohol) membrane. *Fluid Phase Equilibria*, **2011**, 302, 14-20	2.5	19
61	pH-Responsive Zwitterionic Copolymer DHA-PBLG-PCB for Targeted Drug Delivery: A Computer Simulation Study. *Langmuir*, **2019**, 35, 1944-1953	4	19
60	Molecular simulation study of feruloyl esterase adsorption on charged surfaces: effects of surface charge density and ionic strength. *Langmuir*, **2015**, 31, 10751-63	4	18

59	Mesoscopic simulation studies on the formation mechanism of drug loaded polymeric micelles. *Colloids and Surfaces B: Biointerfaces*, **2015**, 136, 536-44	6	18
58	Hydrolysis-controlled protein adsorption and antifouling behaviors of mixed charged self-assembled monolayer: A molecular simulation study. *Acta Biomaterialia*, **2016**, 40, 23-30	10.8	18
57	Electric-Field Effects on Ionic Hydration: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2018**, 122, 5991-5998	3.4	18
56	Atomistic simulations of the solid-liquid transition of 1-ethyl-3-methyl imidazolium bromide ionic liquid. *Journal of Chemical Physics*, **2011**, 135, 144501	3.9	18
55	Preparation of a Nanobiocatalyst by Efficiently Immobilizing Aspergillus niger Lipase onto Magnetic MetalBiomolecule Frameworks (BioMOF). *ChemCatChem*, **2017**, 9, 1794-1800	5.2	17
54	Phase Behavior of an Amphiphilic Block Copolymer in Ionic Liquid: A Dissipative Particle Dynamics Study. *Journal of Chemical & Engineering Data*, **2016**, 61, 3998-4005	2.8	17
53	Zwitterionic Membrane via Nonsolvent Induced Phase Separation: A Computer Simulation Study. *Langmuir*, **2019**, 35, 1973-1983	4	17
52	Mesoscopic Structures of Poly(carboxybetaine) Block Copolymer and Poly(ethylene glycol) Block Copolymer in Solutions. *Langmuir*, **2017**, 33, 7575-7582	4	17
51	Molecular Simulation of Oxygen Sorption and Diffusion in the Poly (lactic acid). *Chinese Journal of Chemical Engineering*, **2013**, 21, 301-309	3.2	17
50	Multiscale modeling and simulations of responsive polymers. *Current Opinion in Chemical Engineering*, **2019**, 23, 21-33	5.4	16
49	Molecular simulations of myoglobin adsorbed on rutile (1 1 0) and (0 0 1) surfaces. *Fluid Phase Equilibria*, **2014**, 362, 349-354	2.5	16
48	Underwater Superoleophobicity of Pseudozwitterionic SAMs: Effects of Chain Length and Ionic Strength. *Journal of Physical Chemistry C*, **2017**, 121, 17390-17401	3.8	16
47	Molecular simulations of lysozyme adsorption on an electrically responsive mixed self-assembled monolayer. *Applied Surface Science*, **2020**, 506, 144962	6.7	15
46	Unprecedented Wiring Efficiency of Sulfonated Graphitic Carbon Nitride Materials: Toward High-Performance Amperometric Recombinant CotA Laccase Biosensors. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 1474-1484	8.3	15
45	Catechol-cation adhesion on silica surfaces: molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2017**, 19, 29222-29231	3.6	14
44	Computer Simulations on the Channel Membrane Formation by Nonsolvent Induced Phase Separation. *Macromolecular Theory and Simulations*, **2017**, 26, 1700027	1.5	14
43	Communication: Molecular dynamics simulations of the interfacial structure of alkali metal fluoride solutions. *Journal of Chemical Physics*, **2010**, 133, 061103	3.9	14
42	Computer Simulations on the Anticancer Drug Delivery System of Docetaxel and PLGA-PEG Copolymer. *Acta Chimica Sinica*, **2012**, 70, 2445	3.3	14

41	Molecular mechanism of HIV-1 TAT peptide and its conjugated gold nanoparticles translocating across lipid membranes. *Physical Chemistry Chemical Physics*, **2019**, 21, 10300-10310	3.6	13
40	Hamiltonian replica exchange simulations of glucose oxidase adsorption on charged surfaces. *Physical Chemistry Chemical Physics*, **2018**, 20, 14587-14596	3.6	13
39	Computer Simulation of DNA Condensation by PAMAM Dendrimer. *Macromolecular Theory and Simulations*, **2018**, 27, 1700070	1.5	13
38	Designing new amine functionalized metal-organic frameworks for carbon dioxide/methane separation. *Fluid Phase Equilibria*, **2014**, 362, 342-348	2.5	13
37	Advanced Monte Carlo simulations of the adsorption of chiral alcohols in a homochiral metal-organic framework. *AICHE Journal*, **2014**, 60, 2324-2334	3.6	13
36	Orientation of a Y-shaped biomolecule adsorbed on a charged surface. *Physical Review E*, **2002**, 66, 011911	1.4	13
35	Computer simulations of the adsorption of an N-terminal peptide of statherin, SN15, and its mutants on hydroxyapatite surfaces. *Physical Chemistry Chemical Physics*, **2019**, 21, 9342-9351	3.6	12
34	Computer Simulations on a pH-Responsive Anticancer Drug Delivery System Using Zwitterion-Grafted Polyamidoamine Dendrimer Unimolecular Micelles. *Langmuir*, **2021**, 37, 1225-1234	4	12
33	Solvent-responsiveness of PS–PEO binary mixed polymer brushes: a coarse-grained molecular dynamics study. *Molecular Simulation*, **2017**, 43, 1322-1330	2	11
32	Enzymatic characterization of a recombinant carbonyl reductase from sp. CCTCC M209061. *Bioresources and Bioprocessing*, **2017**, 4, 39	5.2	10
31	Simulated revelation of the adsorption behaviours of acetylcholinesterase on charged self-assembled monolayers. *Nanoscale*, **2020**, 12, 3701-3714	7.7	10
30	Catechol and Its Derivatives Adhesion on Graphene: Insights from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2018**, 122, 22965-22974	3.8	10
29	Homoporous polymer membrane via forced surface segregation: A computer simulation study. *Chemical Engineering Science*, **2018**, 191, 490-499	4.4	9
28	The application of poly(methyl methacrylate-co-butyl acrylate-co-styrene) in reinforcing fragile papers: experiments and computer simulations. *Cellulose*, **2017**, 24, 5157-5171	5.5	9
27	Interfacial microenvironment for lipase immobilization: Regulating the heterogeneity of graphene oxide. *Chemical Engineering Journal*, **2020**, 394, 125038	14.7	8
26	Two-dimensional self-assembly of esters with different configurations at the liquid–solid interface. *Applied Surface Science*, **2011**, 257, 4559-4565	6.7	8
25	Electrostatic Effect of Functional Surfaces on the Activity of Adsorbed Enzymes: Simulations and Experiments. *ACS Applied Materials & Interfaces*, **2020**, 12, 35676-35687	9.5	6
24	Molecular simulations on the hydration and underwater oleophobicity of zwitterionic self-assembled monolayers. *AICHE Journal*, **2021**, 67, e17103	3.6	6

23	A molecular level performance manipulation of thermal conductivity and moisture diffusivity through a composite membrane considering interfacial resistance. *Journal of Membrane Science*, **2019**, 583, 231-247	9.6	5
22	Computer simulations on double hydrophobic PS-b-PMMA porous membrane by non-solvent induced phase separation. *Fluid Phase Equilibria*, **2020**, 523, 112784	2.5	5
21	A coarse-grained simulation of heat and mass transfer through a graphene oxide-based composite membrane. *Chemical Engineering Science*, **2021**, 243, 116692	4.4	5
20	Molecular thin films on solid surfaces: mechanisms of melting. *Langmuir*, **2012**, 28, 7382-92	4	4
19	Effect of Topology of Hydrophobic Surfaces on Their Wetting States by Coarse-grained Simulations. *Acta Chimica Sinica*, **2014**, 72, 1075	3.3	4
18	Molecular simulations of charged complex fluids: A review. *Chinese Journal of Chemical Engineering*, **2021**, 31, 206-226	3.2	4
17	Computer simulation of zwitterionic polymer brush grafted silica nanoparticles to modify polyvinylidene fluoride membrane. *Journal of Colloid and Interface Science*, **2021**, 587, 173-182	9.3	4
16	Replica Exchange Molecular Dynamics Simulations on the Folding of Trpzip4 Hairpin. *Acta Chimica Sinica*, **2013**, 71, 593	3.3	3
15	Lysozyme Adsorption on Porous Organic Cages: A Molecular Simulation Study. *Langmuir*, **2020**, 36, 12299-12308	4	3
14	Simulation Insight into the Synergic Role of Citrate and Polyaspartic Peptide in Biomineralization. *Langmuir*, **2021**, 37, 3410-3419	4	3
13	Mesoscopic Structure of Nafion-Ionic Liquid Membrane Using Dissipative Particle Dynamics Simulations. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2016**, 32, 1649-1657	3.8	3
12	Computer simulations of underwater oil adhesion of self-assembled monolayers on Au (111). *Molecular Simulation*, **2020**, 46, 713-720	2	3
11	Computer Simulations of Fibronectin Adsorption on Graphene Modified Titanium Dioxide Surfaces. *Acta Chimica Sinica*, **2014**, 72, 401	3.3	2
10	Molecular fingerprint and machine learning to accelerate design of high-performance homochiral metal–organic frameworks. *AICHE Journal*, **2021**, 67, e17352	3.6	2
9	A novel anticaries agent, honokiol-loaded poly(amido amine) dendrimer, for simultaneous long-term antibacterial treatment and remineralization of demineralized enamel. *Dental Materials*, **2021**, 37, 1337-1349	5.7	2
8	ACAP1 assembles into an unusual protein lattice for membrane deformation through multiple stages. *PLoS Computational Biology*, **2019**, 15, e1007081	5	1
7	Surface Structure and Interaction of Surface/Interface Probed by Mesoscale Simulations and Experiments. *Advances in Chemical Engineering*, **2015**, 47, 85-162	0.6	1
6	Dual-responsive zwitterion-modified nanopores: a mesoscopic simulation study.. *Journal of Materials Chemistry B*, **2022**,	7.3	1

5	Simulated preparation and hydration property of a new-generation zwitterionic modified PVDF membrane. *Journal of Membrane Science*, **2022**, 652, 120498	9.6	1
4	The interplay between surface-functionalized gold nanoparticles and negatively charged lipid vesicles. *Physical Chemistry Chemical Physics*, **2021**, 23, 23526-23536	3.6	0
3	Lysozyme Adsorption on Different Functionalized MXenes: A Multiscale Simulation Study. *Langmuir* , **2021**, 37, 5932-5942	4	0
2	Crystallization of Sodium Bicarbonate in the Presence of Trace Amounts of HPMA. *ChemistrySelect*, **2021**, 6, 2184-2188	1.8	0
1	Simulated synthesis of silica nanowires by lyotropic liquid crystal template method. *Molecular Simulation*,1-11	2	