

Shiling Yuan

List of Publications by Year in descending order

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136
papers

2,973
citations

218677

26
h-index

214800

47
g-index

137
all docs

137
docs citations

137
times ranked

3477
citing authors

#	ARTICLE	IF	CITATIONS
1	Atomistic insights into uptake of hydrogen peroxide by TiO ₂ particles as a function of humidity. <i>Journal of Molecular Liquids</i> , 2022, 346, 117097.	4.9	1
2	Molecular dynamics study on emulsified oil droplets with nonionic surfactants. <i>Journal of Molecular Liquids</i> , 2022, 346, 117102.	4.9	15
3	Atomistic insights into heterogeneous reaction of formic acid on mineral oxide particles. <i>Chemosphere</i> , 2022, 287, 132430.	8.2	6
4	Degradation evaluation of acrylamide in advanced oxidation processes based on theoretical method: Mechanisms, kinetics, toxicity evaluation and the role of soil particles. <i>Journal of Hazardous Materials</i> , 2022, 424, 127592.	12.4	12
5	Molecular insights into the uptake of SiO ₂ nanoparticles on phospholipid membrane: Effect of surface properties and particle size. <i>Colloids and Surfaces B: Biointerfaces</i> , 2022, 210, 112250.	5.0	10
6	Mechanistic study of the adsorption and penetration of modified SiO ₂ nanoparticles on cellular membrane. <i>Chemosphere</i> , 2022, 294, 133793.	8.2	7
7	Molecular Dynamics Simulation for the Demulsification of O/W Emulsion under Pulsed Electric Field. <i>Molecules</i> , 2022, 27, 2559.	3.8	3
8	Molecular Dynamics Study on Properties of Hydration Layers above Polymer Antifouling Membranes. <i>Molecules</i> , 2022, 27, 3074.	3.8	6
9	Theoretical insights into the uptake of sulfonamides onto phospholipid bilayers: Mechanisms, interaction and toxicity evaluation. <i>Journal of Hazardous Materials</i> , 2022, 435, 129033.	12.4	10
10	Neolithic burial pottery from the Jiaojia site, China: A multi- $\delta^{13}C$ analytical study. <i>Archaeometry</i> , 2022, 64, 1359-1376.	1.3	0
11	Molecular dynamics simulation of demulsification of O/W emulsion containing soil in direct current electric field. <i>Journal of Molecular Liquids</i> , 2022, 361, 119618.	4.9	6
12	Molecular dynamics study on adsorption and desorption of lysozyme above polymer antifouling membranes. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 649, 129466.	4.7	8
13	Self-assembly of metal nanoclusters in colloid science. , 2022, , 385-407.		0
14	Computational investigation of a switchable emulsion stabilized by the mixture of a surfactant and tertiary amine. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 368-377.	2.8	6
15	Atomistic Insights into Oxidation of Chemical Passivated Silicon (100) Surface: Reactive Molecular Dynamic Simulations. <i>Chinese Journal of Chemistry</i> , 2021, 39, 896-902.	4.9	0
16	Effect of salt-resistant monomers on viscosity of modified polymers based on the hydrolyzed poly-acrylamide (HPAM): A molecular dynamics study. <i>Journal of Molecular Liquids</i> , 2021, 325, 115161.	4.9	35
17	Atomistic insights into resistance to oxidation of Si (111) grafted different organic chains. <i>Computational Materials Science</i> , 2021, 191, 110336.	3.0	4
18	A study of influence factors to improve the heat transfer of pure-polydimethylsiloxane (PDMS): A molecular dynamics study. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 618, 126409.	4.7	11

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19	Atomistic insights into heterogeneous reaction of hydrogen peroxide on mineral oxide particles. <i>Applied Surface Science</i> , 2021, 556, 149707.	6.1	6
20	Determination of Minimum Miscibility Pressure of CO ₂ -Oil System: A Molecular Dynamics Study. <i>Molecules</i> , 2021, 26, 4983.	3.8	4
21	Pseudo-zwitterions self-assembled from polycation and anion clusters showing exceptional water-cleanable anti-crude-oil-adhesion property. <i>IScience</i> , 2021, 24, 102964.	4.1	4
22	Atomistic insights into heterogeneous reaction of hydrogen peroxide on alumina particles: Combining DFT calculation and ReaxFF molecular dynamics simulations. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 626, 127064.	4.7	2
23	Understanding the properties of methyl vinyl ketone and methacrolein at the air-water interface: Adsorption, heterogeneous reaction and environmental impact analysis. <i>Chemosphere</i> , 2021, 283, 131183.	8.2	10
24	Enhanced uptake of methacrolein at the acidic nanoparticle interface: Adsorption, heterogeneous reaction and impact for the secondary organic aerosol formation. <i>Science of the Total Environment</i> , 2021, 800, 149532.	8.0	8
25	Molecular Dynamics Simulation of Thermal Conductivity of Al ₂ O ₃ /PDMS Composites. <i>Acta Chimica Sinica</i> , 2021, 79, 787.	1.4	0
26	Molecular dynamics study on the effect of surfactant mixture on their packing states in mixed micelles. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 631, 127714.	4.7	4
27	Manufacturing techniques of sacrificial pottery from Jiaojia site, China, during the Dawenkou Culture. <i>Journal of Archaeological Science: Reports</i> , 2021, 40, 103238.	0.5	2
28	Compound Cleaning Agent for Oily Sludge from Experiments and Molecular Simulations. <i>ACS Omega</i> , 2021, 6, 33300-33309.	3.5	2
29	Reactive Molecular Dynamics on the Oxidation of H ₂ -Si(100) Surface: Effect of Humidity and Temperature. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1932-1940.	3.1	13
30	Photothermally triggered cytosolic drug delivery of glucose functionalized polydopamine nanoparticles in response to tumor microenvironment for the GLUT1-targeting chemo-phototherapy. <i>Journal of Controlled Release</i> , 2020, 317, 232-245.	9.9	63
31	A Green Solvent Processable Wide-Bandgap Conjugated Polymer for Organic Solar Cells. <i>Solar Rrl</i> , 2020, 4, 2000547.	5.8	13
32	Exploring relationship of the state of N-dodecyl betaine in the solution monomer, at the interface and in the micelle via configurational entropy. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 600, 124975.	4.7	4
33	Molecular Dynamics Study on the Adsorption of Heavy Oil Drops on a Silica Surface with Different Hydrophobicity. <i>Energy & Fuels</i> , 2020, 34, 7019-7028.	5.1	19
34	Emulsification of Surfactant on Oil Droplets by Molecular Dynamics Simulation. <i>Molecules</i> , 2020, 25, 3008.	3.8	16
35	Reactive molecular dynamics on the oxidation of passivated H-terminated Si (111) surface: 1-Alkynes vs 1-Alkenes. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 606, 125372.	4.7	5
36	RADIOCARBON DATING AND DIET: THE JIAOJIA SITE IN CHINA. <i>Radiocarbon</i> , 2020, 62, 1515-1523.	1.8	5

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37	Molecular Dynamics Study on the Suitable Compatibility Conditions of a CO ₂ -Cosolvent-Light Hydrocarbon System by Calculating the Solubility Parameters. <i>Energy & Fuels</i> , 2020, 34, 3483-3492.	5.1	8
38	Ultrathin Supramolecular Architectures Self-Assembled from a C ₃ -Symmetric Synthon for Selective Metal Binding. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 9673-9681.	8.0	4
39	Molecular dynamics studies on the aggregating behaviors of cellulose molecules in NaOH/urea aqueous solution. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 594, 124663.	4.7	21
40	Gaseous and heterogeneous reactions of low-molecular-weight (LMW) unsaturated ketones with O ₃ : Mechanisms, kinetics, and effects of mineral dust in tropospheric chemical processes. <i>Chemical Engineering Journal</i> , 2020, 395, 125083.	12.7	27
41	Four Methods to Estimate Minimum Miscibility Pressure of CO ₂ -Oil Based on Machine Learning. <i>Chinese Journal of Chemistry</i> , 2019, 37, 1271-1278.	4.9	19
42	Adsorption of C ₅ Pe molecules on silica surfaces with different hydrophobicity studied by molecular dynamics simulation. <i>Applied Surface Science</i> , 2019, 495, 143624.	6.1	26
43	Amphiphilicity Regulation of Ag ^I Nanoclusters: Self-Assembly and Its Application as a Luminescent Probe. <i>Chemistry - A European Journal</i> , 2019, 25, 4713-4721.	3.3	24
44	Effect of SDS on Reducing the Viscosity of Heavy Oil: A Molecular Dynamics Study. <i>Energy & Fuels</i> , 2019, 33, 4921-4930.	5.1	19
45	A molecular dynamics study combining with entropy calculation on the packing state of hydrophobic chains in micelle interior. <i>Journal of Molecular Liquids</i> , 2019, 283, 860-866.	4.9	7
46	Synergistic Adsorption of Polyaromatic Compounds on Silica Surfaces Studied by Molecular Dynamics Simulation. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4290-4299.	3.1	27
47	A molecular dynamics study of cellulose inclusion complexes in NaOH/urea aqueous solution. <i>Carbohydrate Polymers</i> , 2018, 185, 12-18.	10.2	14
48	pH-Responsive Nanovesicles with Enhanced Emission Co-Assembled by Ag(I) Nanoclusters and Polyethyleneimine as a Superior Sensor for Al ³⁺ . <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 3955-3963.	8.0	94
49	The mechanism of restructuring of surfactant monolayer on mica surface in aqueous solution: molecular dynamics simulation. <i>Molecular Simulation</i> , 2018, 44, 396-404.	2.0	6
50	Zwitterionic polymers functionalised nanoporous graphene for water desalination: a molecular dynamics study. <i>Molecular Simulation</i> , 2018, 44, 349-357.	2.0	4
51	Molecular Dynamics Study on Aggregating Behavior of Asphaltene and Resin in Emulsified Heavy Oil Droplets with Sodium Dodecyl Sulfate. <i>Energy & Fuels</i> , 2018, 32, 12383-12393.	5.1	68
52	Realizing enhanced luminescence of silver nanocluster-peptide soft hydrogels by PEI reinforcement. <i>Soft Matter</i> , 2018, 14, 8352-8360.	2.7	16
53	A molecular dynamics study on the dependence of phase behaviors and structural properties of two-dimensional interfacial monolayer on surface area. <i>Applied Surface Science</i> , 2018, 459, 741-748.	6.1	5
54	Molecular dynamics simulation of thickening mechanism of supercritical CO ₂ thickener. <i>Chemical Physics Letters</i> , 2018, 706, 658-664.	2.6	14

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55	Self-Assembled Minimalist Multifunctional Theranostic Nanoplatform for Magnetic Resonance Imaging-Guided Tumor Photodynamic Therapy. <i>ACS Nano</i> , 2018, 12, 8266-8276.	14.6	191
56	The cloud point phenomenon of ionic surfactants: A view from molecular dynamics and metadynamics simulation. <i>Journal of Molecular Liquids</i> , 2018, 269, 298-303.	4.9	0
57	Decomposition of CH ₄ hydrate: effects of temperature and salt from molecular simulations. <i>Molecular Simulation</i> , 2018, 44, 1220-1228.	2.0	18
58	Influence of functional groups on water splitting in carbon nanodot and graphitic carbon nitride composites: a theoretical mechanism study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4997-5003.	2.8	34
59	The effect of betaine on the foam stability: Molecular simulation. <i>Applied Surface Science</i> , 2017, 407, 156-161.	6.1	27
60	Structural changes of PMMA substrates with different electrolyte solutions: A molecular dynamics study. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2017, 522, 51-57.	4.7	3
61	Adsorption of a Polyaromatic Compound on Silica Surfaces from Organic Solvents Studied by Molecular Dynamics Simulation and AFM Imaging. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5020-5028.	3.1	65
62	Electronic structures of rutile (011)(2 Å ⁻¹) surfaces: A many-body perturbation theory study. <i>Journal of Chemical Physics</i> , 2017, 146, 124702.	3.0	6
63	Molecular dynamics study on oil migration inside silica nanopore. <i>Chemical Physics Letters</i> , 2017, 678, 186-191.	2.6	16
64	The properties of asphaltene at the oil-water interface: A molecular dynamics simulation. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2017, 515, 34-40.	4.7	45
65	A molecular dynamics study on the adsorption of a mussel protein on two different films: Polymer film and a SAM. <i>Chemical Physics Letters</i> , 2017, 676, 144-149.	2.6	6
66	Ionic Self-Assembly of Polyoxometalate-Dopamine Hybrid Nanoflowers with Excellent Catalytic Activity for Dyes. <i>ACS Sustainable Chemistry and Engineering</i> , 2017, 5, 1358-1367.	6.7	65
67	Formation of organogels with aggregation-induced emission characteristics triggered by thermal and ultrasound. <i>Colloid and Polymer Science</i> , 2017, 295, 1765-1772.	2.1	6
68	Molecular dynamics simulation of sodium dodecylsulfate (SDS) bilayers. <i>Journal of Colloid and Interface Science</i> , 2017, 506, 227-235.	9.4	15
69	Molecular dynamics study on mechanism of preformed particle gel transporting through nanopores: Surface chemistry and heterogeneity. <i>Chemical Physics Letters</i> , 2017, 685, 294-299.	2.6	5
70	Self-assembly of water-soluble silver nanoclusters: superstructure formation and morphological evolution. <i>Nanoscale</i> , 2017, 9, 19191-19200.	5.6	56
71	Self-Assembly of Peptide-Polyoxometalate Hybrid Sub-Micrometer Spheres for Photocatalytic Degradation of Methylene Blue. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10566-10573.	2.6	26
72	MesoDyn prediction of a pharmaceutical microemulsion self-assembly consistent with experimental measurements. <i>RSC Advances</i> , 2017, 7, 20293-20299.	3.6	7

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73	A Robust Polyionized Hydrogel with an Unprecedented Underwater Anti-Crude Oil Adhesion Property. <i>Advanced Materials</i> , 2016, 28, 5307-5314.	21.0	346
74	Molecular dynamics study on the aggregation behaviour of different positional isomers of sodium dodecyl benzenesulphonate. <i>RSC Advances</i> , 2016, 6, 49708-49716.	3.6	13
75	Self-assembled chiral helical nanofibers by amphiphilic dipeptide derived from d - or l -threonine and application as a template for the synthesis of Au and Ag nanoparticles. <i>Journal of Colloid and Interface Science</i> , 2016, 484, 97-106.	9.4	28
76	A molecular dynamics study on two promising green surfactant micelles of choline dodecyl sulfate and laurate. <i>RSC Advances</i> , 2016, 6, 84090-84097.	3.6	18
77	The formation and stability of sodium dodecylsulfate vesicles mediated by rough glass surface. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2016, 509, 195-202.	4.7	8
78	Molecular dynamics simulations on tetraalkylammonium interactions with dodecyl sulfate micelles at the air/water interface. <i>Journal of Molecular Liquids</i> , 2016, 222, 1085-1090.	4.9	16
79	Molecular Dynamics Study on Mechanism of Preformed Particle Gel Transporting Through Nanopores: Deformation and Dehydration. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19389-19395.	3.1	9
80	Ionic Self-Assembly of a Giant Vesicle as a Smart Microcarrier and Microreactor. <i>Langmuir</i> , 2016, 32, 9548-9556.	3.5	26
81	Fabrication of Smart pH-Responsive Fluorescent Solid-like Giant Vesicles by Ionic Self-Assembly Strategy. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27533-27540.	3.1	30
82	Tunable Aggregation-Induced Emission of Polyoxometalates via Amino Acid-Directed Self-Assembly and Their Application in Detecting Dopamine. <i>Langmuir</i> , 2016, 32, 13736-13745.	3.5	49
83	A kinetic Monte Carlo simulation of center shift on template-induced surface. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2016, 509, 401-407.	4.7	1
84	Molecular Dynamics Simulation of the Oil Detachment Process within Silica Nanopores. <i>Journal of Physical Chemistry C</i> , 2016, 120, 2667-2674.	3.1	55
85	Manipulation the properties of supramolecular hydrogels of β -cyclodextrin/Tyloxapol/carbon-based nanomaterials. <i>Journal of Colloid and Interface Science</i> , 2016, 468, 78-85.	9.4	19
86	Ultrasensitive detection of aliphatic nitro-organics based on "turn-on" fluorescent sensor array. <i>Science China Chemistry</i> , 2016, 59, 89-94.	8.2	10
87	Molecular dynamics study on mechanism of preformed particle gel transporting through nanopores: surface hydration. <i>RSC Advances</i> , 2016, 6, 7172-7180.	3.6	11
88	A kinetic Monte Carlo simulation of organic particles hetero-patterning on template-induced surface. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2016, 494, 186-193.	4.7	2
89	Origins of entropy change for the amphiphilic molecule in micellization: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11357-11361.	2.8	9
90	Smart stimuli-responsive fluorescent vesicular sensor based on inclusion complexation of cyclodextrins with Tyloxapol. <i>RSC Advances</i> , 2016, 6, 11683-11690.	3.6	7

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91	Modulating self-assembly behavior of a salt-free peptide amphiphile (PA) and zwitterionic surfactant mixed system. <i>Journal of Colloid and Interface Science</i> , 2016, 467, 43-50.	9.4	23
92	Modulating hierarchical self-assembly behavior of a peptide amphiphile/nonionic surfactant mixed system. <i>RSC Advances</i> , 2016, 6, 9186-9193.	3.6	12
93	Tetraalkylammonium interactions with dodecyl sulfate micelles: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 878-885.	2.8	19
94	Incorporation of graphene oxide into C ₁₂ E ₄ /C ₁₂ mimBr hybrid lyotropic liquid crystal and its thermo-sensitive properties. <i>RSC Advances</i> , 2015, 5, 68404-68412.	3.6	10
95	The mechanism of selective deposition of luminescent molecules onto self-assembled monolayers using molecular dynamics. <i>Applied Surface Science</i> , 2015, 349, 163-168.	6.1	8
96	A kinetic Monte Carlo simulation of surface microfluidic patterning organic molecules based on anisotropic wetting. <i>Chemical Physics Letters</i> , 2015, 628, 54-59.	2.6	4
97	Low temperature molecular dynamic simulation of water structure at sylvite crystal surface in saturated solution. <i>Minerals Engineering</i> , 2015, 83, 53-58.	4.3	32
98	Effects of graphene oxide and salinity on sodium deoxycholate hydrogels and their applications in dye absorption. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2015, 483, 112-120.	4.7	14
99	Self-assembly of dipeptide sodium salts derived from alanine: a molecular dynamics study. <i>RSC Advances</i> , 2015, 5, 102182-102190.	3.6	22
100	Mechanism of oil detachment from hybrid hydrophobic and hydrophilic surface in aqueous solution. <i>Journal of Chemical Physics</i> , 2014, 140, 164702.	3.0	33
101	Synthesis, characterization, and evaluation of TiMgAlCu mixed oxides as novel SO _x removal catalysts. <i>Ceramics International</i> , 2014, 40, 11559-11566.	4.8	7
102	C and N stable isotope analysis of human and animal bones at the Beiqian site. <i>Science China Earth Sciences</i> , 2014, 57, 408-414.	5.2	2
103	Molecular dynamics study of the structure of an oppositely charged polyelectrolyte and an ionic surfactant at the air/water interface. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2014, 454, 104-112.	4.7	22
104	Molecular Dynamics Simulation: The Behavior of Asphaltene in Crude Oil and at the Oil/Water Interface. <i>Energy & Fuels</i> , 2014, 28, 7368-7376.	5.1	124
105	Ordered carbon nanotubes/n-dodecyl tetraethylene monoether liquid crystal composites through phase separation induced by poly(ethylene glycol). <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14771-14780.	2.8	16
106	Aggregation Behavior of Trisiloxane-Tailed Surface Active Ionic Liquids in Aqueous Solution: Coarse-Grained Molecular Dynamics Study. <i>Journal of Dispersion Science and Technology</i> , 2014, 35, 1520-1527.	2.4	8
107	Comparative study of n-dodecyl tetraethylene monoether lyotropic liquid crystals incorporated with graphene and graphene oxide. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20932-20940.	2.8	19
108	Mechanism of foam destruction by antifoams: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17231.	2.8	23

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109	Molecular dynamics study of the adsorption of anionic surfactant in a nonionic polymer brush. <i>Journal of Molecular Modeling</i> , 2014, 20, 2267.	1.8	7
110	Step-edge induced area selective growth: a kinetic Monte Carlo study. <i>RSC Advances</i> , 2014, 4, 25005-25010.	3.6	6
111	Influence of self-assembled monolayers on the growth and crystallization of rubrene films: a molecular dynamics study. <i>RSC Advances</i> , 2013, 3, 15404.	3.6	8
112	Deposition behavior onto different template structures and step-edge induced area-selective growth of rubrene: A molecular dynamics study. <i>Chemical Physics Letters</i> , 2013, 571, 38-43.	2.6	7
113	Facile synthesis of hierarchically porous silica nanocapsules and nanospheres via vesicle templating. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2013, 424, 59-65.	4.7	12
114	Properties of a water layer on hydrophilic and hydrophobic self-assembled monolayer surfaces: A molecular dynamics study. <i>Science China Chemistry</i> , 2013, 56, 773-781.	8.2	23
115	A molecular dynamics simulation of N-(fluorenyl-9-methoxycarbonyl)-dipeptides supramolecular hydrogel. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2013, 417, 217-223.	4.7	20
116	Fluorescent probe solubilised in cetyltrimethylammonium bromide micelles by molecular dynamics simulation. <i>Molecular Simulation</i> , 2013, 39, 1042-1051.	2.0	6
117	Coarse-grained molecular dynamics simulation of self-assembly of polyacrylamide and sodium dodecylsulfate in aqueous solution. <i>Journal of Colloid and Interface Science</i> , 2012, 386, 205-211.	9.4	31
118	Mechanism of Oil Detachment from a Silica Surface in Aqueous Surfactant Solutions: Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2867-2875.	2.6	105
119	Reconstructing the food structure of ancient coastal inhabitants from Beiqian village: Stable isotopic analysis of fossil human bone. <i>Science Bulletin</i> , 2012, 57, 2148-2154.	1.7	11
120	Mesoscopic simulation on phase behavior of star-like block polyether solution in the absence and presence of shear. <i>Soft Matter</i> , 2011, 7, 9035.	2.7	4
121	Selective deposition of organic molecules onto different densely packed self-assembled monolayers: A molecular dynamics study. <i>Chemical Physics Letters</i> , 2011, 507, 138-143.	2.6	17
122	Molecular Dynamics Study of Alkyl Benzene Sulfonate at Air/Water Interface: Effect of Inorganic Salts. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5025-5033.	2.6	100
123	Mesoscopic simulation studies on micellar phases of Pluronic P103 solution. <i>Journal of Molecular Modeling</i> , 2008, 14, 607-620.	1.8	11
124	Phase behavior of tri-block copolymers in solution: Mesoscopic simulation study. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2008, 322, 87-96.	4.7	21
125	Mesoscopic Simulation of the Phase Separation on Triblock Copolymer in Aqueous Solution. <i>Acta Physico-chimica Sinica</i> , 2007, 23, 139-144.	0.6	7
126	Theoretical study on reactions of alkene molecules on H-terminated Si(111): Density functional theory and ab initio molecular dynamics. <i>Chemical Physics Letters</i> , 2007, 438, 53-58.	2.6	7

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127	Interaction between dodecyl oxypropyl $\hat{2}$ -hydroxytrimethylammonium bromide and Xanthan: MesoDyn simulation and binding isotherm measurements. <i>Science Bulletin</i> , 2007, 52, 2605-2611.	1.7	1
128	Mesoscopic Simulation on Phase Behavior of Ternary Copolymeric Solution in the Absence and Presence of Shear. <i>Macromolecules</i> , 2006, 39, 6631-6642.	4.8	29
129	Molecular dynamics studies on octadecylammonium chloride at the air/liquid interface. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2006, 280, 108-115.	4.7	10
130	Molecular dynamics studies on monolayer of cetyltrimethylammonium bromide surfactant formed at the air/water interface. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2006, 289, 1-9.	4.7	61
131	Property Prediction on Surfactant by Quantitative Structure-Property Relationship: Krafft Point and Cloud Point. <i>Journal of Dispersion Science and Technology</i> , 2005, 26, 799-808.	2.4	16
132	Molecular simulation study of different monolayers on Si (111) surface. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2004, 242, 129-135.	4.7	21
133	The Effect of Macromolecules on Foam Stability in Sodium Dodecyl Sulfate/Cetylpyridinium Bromide Mixtures. <i>Journal of Dispersion Science and Technology</i> , 2003, 24, 779-787.	2.4	21
134	Quantitative Structure-Property Relationships of Surfactants: Critical Micelle Concentration of Anionic Surfactants. <i>Journal of Dispersion Science and Technology</i> , 2002, 23, 465-472.	2.4	19
135	Quantitative structure-property relationships of surfactants: prediction of the critical micelle concentration of nonionic surfactants. <i>Colloid and Polymer Science</i> , 2002, 280, 630-636.	2.1	19
136	Effect of Polyvinylpyrrolidone on the States of Water in Water-in-Oil Microemulsions with Betaine Surfactant. <i>Journal of Dispersion Science and Technology</i> , 2001, 22, 563-567.	2.4	4