Jian Zhou

List of Publications by Year
in descending order

133 papers	5,482 citations	66234 42 h-index	98622 67 g-index
136 all docs	136 docs citations	136 times ranked	6242 citing authors

#	Article	IF	Citations
1	Controlling Antibody Orientation on Charged Self-Assembled Monolayers. Langmuir, 2003, 19, 2859-2864.	1.6	232
2	Bioinspired Graphene Nanopores with Voltage-Tunable Ion Selectivity for Na⁺ and K⁺. ACS Nano, 2013, 7, 10148-10157.	7.3	199
3	An ethane-trapping MOF PCN-250 for highly selective adsorption of ethane over ethylene. Chemical Engineering Science, 2018, 175, 110-117.	1.9	177
4	Coarse-Grained Peptide Modeling Using a Systematic Multiscale Approach. Biophysical Journal, 2007, 92, 4289-4303.	0.2	176
5	Molecular dynamics study on ionic hydration. Fluid Phase Equilibria, 2002, 194-197, 257-270.	1.4	161
6	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.	1.2	145
7	Diameter and helicity effects on static properties of water molecules confined in carbon nanotubes. Physical Chemistry Chemical Physics, 2004, 6, 829.	1.3	144
8	Orientation of Adsorbed Antibodies on Charged Surfaces by Computer Simulation Based on a United-Residue Model. Langmuir, 2003, 19, 3472-3478.	1.6	129
9	Anomalous Hydration Shell Order of Na⁺ and K⁺ inside Carbon Nanotubes. Nano Letters, 2009, 9, 989-994.	4.5	113
10	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.	5.2	103
11	Monte Carlo simulations of antibody adsorption and orientation on charged surfaces. Journal of Chemical Physics, 2004, 121, 1050-1057.	1.2	100
12	High-throughput computational screening of 137953 metalâ€“organic frameworks for membrane separation of a CO₂/N₂/CH₄ mixture. Journal of Materials Chemistry A, 2016, 4, 15904-15912.	5.2	99
13	Noble Gas Adsorption in Copper Trimesate, HKUST-1: An Experimental and Computational Study. Journal of Physical Chemistry C, 2013, 117, 20116-20126.	1.5	92
14	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 Lennardâ€“Jones fluid. Fluid Phase Equilibria, 2002, 194-197, 1141-1159.	1.4	83
15	Peptide Folding Using Multiscale Coarse-Grained Models. Journal of Physical Chemistry B, 2008, 112, 13079-13090.	1.2	83
16	Parallel tempering Monte Carlo simulations of lysozyme orientation on charged surfaces. Journal of Chemical Physics, 2010, 132, 065101.	1.2	82
17	Probing carbon nanotubeâ€“amino acid interactions in aqueous solution with molecular dynamics simulations. Carbon, 2014, 78, 500-509.	5.4	78
18	Lipase adsorption on different nanomaterials: a multi-scale simulation study. Physical Chemistry Chemical Physics, 2015, 17, 840-850.	1.3	78

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19	Molecular simulation study of temperature effect on ionic hydration in carbon nanotubes. Physical Chemistry Chemical Physics, 2008, 10, 1896.	1.3	76
20	Design of amine-functionalized metalâ€“organic frameworks for CO₂ separation: the more amine, the better?. Chemical Communications, 2016, 52, 974-977.	2.2	76
21	Adsorption of Hydrophobin on Different Self-Assembled Monolayers: The Role of the Hydrophobic Dipole and the Electric Dipole. Langmuir, 2014, 30, 11401-11411.	1.6	68
22	Phase Behavior of Mixed Self-Assembled Monolayers of Alkanethiols on Au(111):Â A Configurational-Bias Monte Carlo Simulation Study. Langmuir, 2001, 17, 7566-7572.	1.6	67
23	Mesoscopic Coarse-Grained Simulations of Lysozyme Adsorption. Journal of Physical Chemistry B, 2014, 118, 4451-4460.	1.2	66
24	Multiscale modeling and simulations of protein adsorption: progresses and perspectives. Current Opinion in Colloid and Interface Science, 2019, 41, 74-85.	3.4	65
25	Ferroelectric Ordering in Ice Nanotubes Confined in Carbon Nanotubes. Nano Letters, 2008, 8, 2607-2612.	4.5	64
26	Ice-like Water Structure in Carbon Nanotube (8,8) Induces Cationic Hydration Enhancement. Journal of Physical Chemistry C, 2013, 117, 11412-11420.	1.5	64
27	Effect of composition on the formation of poly(dl-lactide) microspheres for drug delivery systems: Mesoscale simulations. Chemical Engineering Journal, 2007, 131, 195-201.	6.6	63
28	Adsorption and Diffusion of Supercritical Carbon Dioxide in Slit Pores. Langmuir, 2000, 16, 8063-8070.	1.6	61
29	Diffusion of water molecules confined in slits of rutile TiO2(110) and graphite(0001). Fluid Phase Equilibria, 2011, 302, 316-320.	1.4	59
30	Selective Adsorption of Light Alkanes on a Highly Robust Indium Based Metalâ€“Organic Framework. Industrial & Engineering Chemistry Research, 2017, 56, 4488-4495.	1.8	59
31	Effects of external electric fields on lysozyme adsorption by molecular dynamics simulations. Biophysical Chemistry, 2013, 179, 26-34.	1.5	58
32	Unusual Moisture-Enhanced CO₂ Capture within Microporous PCN-250 Frameworks. ACS Applied Materials & Interfaces, 2018, 10, 38638-38647.	4.0	57
33	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, 23500-23507.	1.3	56
34	Multiscale Simulations of Protein G B1 Adsorbed on Charged Self-Assembled Monolayers. Langmuir, 2013, 29, 11366-11374.	1.6	54
35	Molecular Understanding of the Penetration of Functionalized Gold Nanoparticles into Asymmetric Membranes. Langmuir, 2017, 33, 361-371.	1.6	51
36	Molecular simulations on nanoconfined water molecule behaviors for nanoporous material applications. Microfluidics and Nanofluidics, 2013, 15, 191-205.	1.0	49

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37	Computer simulations of fibronectin adsorption on hydroxyapatite surfaces. RSC Advances, 2014, 4, 15759.	1.7	49
38	Molecular Dynamics Study on Diameter Effect in Structure of Ethanol Molecules Confined in Single-Walled Carbon Nanotubesâ€. Journal of Physical Chemistry C, 2007, 111, 15677-15685.	1.5	48
39	Molecular dynamics simulations of peptide adsorption on self-assembled monolayers. Applied Surface Science, 2012, 258, 8153-8159.	3.1	48
40	Replica-Exchange Molecular Dynamics Simulation of Basic Fibroblast Growth Factor Adsorption on Hydroxyapatite. Journal of Physical Chemistry B, 2014, 118, 5843-5852.	1.2	48
41	Molecular dynamics simulations of conformation changes of HIV-1 regulatory protein on graphene. Applied Surface Science, 2016, 377, 324-334.	3.1	48
42	Ribonuclease A adsorption onto charged self-assembled monolayers: A multiscale simulation study. Chemical Engineering Science, 2015, 121, 331-339.	1.9	45
43	Protein Translocation through a MoS₂ Nanopore:A Molecular Dynamics Study. Journal of Physical Chemistry C, 2018, 122, 2070-2080.	1.5	45
44	Effect of water content on microstructures and oxygen permeation in PSiMAâ€“IPNâ€“PMPC hydrogel: a molecular simulation study. Chemical Engineering Science, 2012, 78, 236-245.	1.9	44
45	Molecular dynamics simulations on the melting of gold nanoparticles. Phase Transitions, 2014, 87, 59-70.	0.6	42
46	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.	2.5	41
47	Self-assembled core-shell and Janus microphase separated structures of polymer blends in aqueous solution. Journal of Chemical Physics, 2013, 139, 084907.	1.2	40
48	Simulation insight into the cytochrome c adsorption on graphene and graphene oxide surfaces. Applied Surface Science, 2018, 428, 825-834.	3.1	39
49	Molecular dynamics investigation on the infinite dilute diffusion coefficients of organic compounds in supercritical carbon dioxide. Fluid Phase Equilibria, 2000, 172, 279-291.	1.4	37
50	Molecular Understanding on the Underwater Oleophobicity of Self-Assembled Monolayers: Zwitterionic versus Nonionic. Langmuir, 2017, 33, 1732-1741.	1.6	37
51	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.	2.4	37
52	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.	3.1	36
53	Electric-Field Effects on Ionic Hydration: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2018, 122, 5991-5998.	1.2	36
54	Solventâ€Responsive Behavior of Polymerâ€Brushâ€Modified Amphiphilic Gold Nanoparticles. Macromolecular Theory and Simulations, 2013, 22, 174-186.	0.6	35

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55	Mesoscopic coarseâ€grained simulations of hydrophobic charge induction chromatography (HCIC) for protein purification. AIChE Journal, 2015, 61, 2035-2047.	1.8	35
56	Electrostatics-mediated Î±-chymotrypsin inhibition by functionalized single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2017, 19, 986-995.	1.3	35
57	Magnetic ZIF-8/cellulose/Fe3O4 nanocomposite: preparation, characterization, and enzyme immobilization. Bioresources and Bioprocessing, 2017, 4, .	2.0	35
58	Computer Simulations on a pH-Responsive Anticancer Drug Delivery System Using Zwitterion-Grafted Polyamidoamine Dendrimer Unimolecular Micelles. Langmuir, 2021, 37, 1225-1234.	1.6	33
59	Bilirubin Oxidase Adsorption onto Charged Self-Assembled Monolayers: Insights from Multiscale Simulations. Langmuir, 2018, 34, 9818-9828.	1.6	32
60	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.	1.5	29
61	Molecular simulations of cytochrome c adsorption on positively charged surfaces: the influence of anion type and concentration. Physical Chemistry Chemical Physics, 2016, 18, 9979-9989.	1.3	29
62	Molecular Understanding of Laccase Adsorption on Charged Self-Assembled Monolayers. Journal of Physical Chemistry B, 2017, 121, 10610-10617.	1.2	29
63	Understanding the Cellular Uptake of pH-Responsive Zwitterionic Gold Nanoparticles: A Computer Simulation Study. Langmuir, 2017, 33, 14480-14489.	1.6	29
64	Interfacial microenvironment for lipase immobilization: Regulating the heterogeneity of graphene oxide. Chemical Engineering Journal, 2020, 394, 125038.	6.6	28
65	Ionic Liquid Confined in Nafion: Toward Molecularâ€Level Understanding. AIChE Journal, 2013, 59, 2630-2639.	1.8	27
66	Lysozyme orientation and conformation on MoS2 surface: Insights from molecular simulations. Biointerphases, 2017, 12, 02D416.	0.6	27
67	pH-Responsive Zwitterionic Copolymer DHAâ€“PBLGâ€“PCB for Targeted Drug Delivery: A Computer Simulation Study. Langmuir, 2019, 35, 1944-1953.	1.6	27
68	Unbinding of the streptavidin-biotin complex by atomic force microscopy: A hybrid simulation study. Journal of Chemical Physics, 2006, 125, 104905.	1.2	26
69	Electrostatic Effect of Functional Surfaces on the Activity of Adsorbed Enzymes: Simulations and Experiments. ACS Applied Materials & Interfaces, 2020, 12, 35676-35687.	4.0	26
70	Interfacial and Phase Transfer Behaviors of Polymer Brush Grafted Amphiphilic Nanoparticles: A Computer Simulation Study. Langmuir, 2014, 30, 5599-5608.	1.6	25
71	Structural properties of polymer-brush-grafted gold nanoparticles at the oilâ€“water interface: insights from coarse-grained simulations. Soft Matter, 2016, 12, 3352-3359.	1.2	25
72	Preparation of a Nanobiocatalyst by Efficiently Immobilizing Aspergillus niger Lipase onto Magnetic Metalâ€“Biomolecule Frameworks (BioMOF). ChemCatChem, 2017, 9, 1794-1800.	1.8	25

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73	Multiscale modeling and simulations of responsive polymers. Current Opinion in Chemical Engineering, 2019, 23, 21-33.	3.8	25
74	Simulated revelation of the adsorption behaviours of acetylcholinesterase on charged self-assembled monolayers. Nanoscale, 2020, 12, 3701-3714.	2.8	25
75	Hydrolysis-controlled protein adsorption and antifouling behaviors of mixed charged self-assembled monolayer: A molecular simulation study. Acta Biomaterialia, 2016, 40, 23-30.	4.1	24
76	Molecular simulations of lysozyme adsorption on an electrically responsive mixed self-assembled monolayer. Applied Surface Science, 2020, 506, 144962.	3.1	24
77	Structures and properties of PAMAM dendrimer: A multi-scale simulation study. Fluid Phase Equilibria, 2011, 302, 43-47.	1.4	23
78	Molecular mechanism of HIV-1 TAT peptide and its conjugated gold nanoparticles translocating across lipid membranes. Physical Chemistry Chemical Physics, 2019, 21, 10300-10310.	1.3	23
79	A mechanical nanogate based on a carbon nanotube for reversible control of ion conduction. Nanoscale, 2014, 6, 3686-3694.	2.8	22
80	Zwitterionic Membrane via Nonsolvent Induced Phase Separation: A Computer Simulation Study. Langmuir, 2019, 35, 1973-1983.	1.6	22
81	Molecular simulation on the separation of water/ethanol azeotropic mixture by poly(vinyl alcohol) membrane. Fluid Phase Equilibria, 2011, 302, 14-20.	1.4	21
82	Molecular Simulation of Oxygen Sorption and Diffusion in the Poly (lactic acid). Chinese Journal of Chemical Engineering, 2013, 21, 301-309.	1.7	21
83	Molecular Simulation Study of Feruloyl Esterase Adsorption on Charged Surfaces: Effects of Surface Charge Density and Ionic Strength. Langmuir, 2015, 31, 10751-10763.	1.6	21
84	Phase Behavior of an Amphiphilic Block Copolymer in Ionic Liquid: A Dissipative Particle Dynamics Study. Journal of Chemical & Engineering Data, 2016, 61, 3998-4005.	1.0	21
85	Underwater Superoleophobicity of Pseudozwitterionic SAMs: Effects of Chain Length and Ionic Strength. Journal of Physical Chemistry C, 2017, 121, 17390-17401.	1.5	21
86	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.	3.2	21
87	Mesoscopic simulation studies on the formation mechanism of drug loaded polymeric micelles. Colloids and Surfaces B: Biointerfaces, 2015, 136, 536-544.	2.5	20
88	Computer Simulations on the Channel Membrane Formation by Nonsolvent Induced Phase Separation. Macromolecular Theory and Simulations, 2017, 26, 1700027.	0.6	20
89	Atomistic simulations of the solid-liquid transition of 1-ethyl-3-methyl imidazolium bromide ionic liquid. Journal of Chemical Physics, 2011, 135, 144501.	1.2	19
90	Molecular simulations of myoglobin adsorbed on rutile (110) and (001) surfaces. Fluid Phase Equilibria, 2014, 362, 349-354.	1.4	19

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91	Mesoscopic Structures of Poly(carboxybetaine) Block Copolymer and Poly(ethylene glycol) Block Copolymer in Solutions. Langmuir, 2017, 33, 7575-7582.	1.6	19
92	Catechol and Its Derivatives Adhesion on Graphene: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 22965-22974.	1.5	19
93	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.	1.3	19
94	Catecholâ€“cation adhesion on silica surfaces: molecular dynamics simulations. Physical Chemistry Chemical Physics, 2017, 19, 29222-29231.	1.3	18
95	Hamiltonian replica exchange simulations of glucose oxidase adsorption on charged surfaces. Physical Chemistry Chemical Physics, 2018, 20, 14587-14596.	1.3	17
96	Computer Simulation of DNA Condensation by PAMAM Dendrimer. Macromolecular Theory and Simulations, 2018, 27, 1700070.	0.6	17
97	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.	1.6	16
98	Designing new amine functionalized metal-organic frameworks for carbon dioxide/methane separation. Fluid Phase Equilibria, 2014, 362, 342-348.	1.4	15
99	Molecular fingerprint and machine learning to accelerate design of <scp>highâ€performance</scp> homochiral metalâ€“organic frameworks. AICHE Journal, 2021, 67, e17352.	1.8	15
100	Computer Simulations on the Anticancer Drug Delivery System of Docetaxel and PLGA-PEG Copolymer. Acta Chimica Sinica, 2012, 70, 2445.	0.5	15
101	Orientation of a Y-shaped biomolecule adsorbed on a charged surface. Physical Review E, 2002, 66, 011911.	0.8	14
102	Communication: Molecular dynamics simulations of the interfacial structure of alkali metal fluoride solutions. Journal of Chemical Physics, 2010, 133, 061103.	1.2	14
103	Advanced Monte Carlo simulations of the adsorption of chiral alcohols in a homochiral metalâ€organic framework. AICHE Journal, 2014, 60, 2324-2334.	1.8	14
104	Solvent-responsiveness of PSâ€“PEO binary mixed polymer brushes: a coarse-grained molecular dynamics study. Molecular Simulation, 2017, 43, 1322-1330.	0.9	14
105	Molecular simulations on the hydration and underwater oleophobicity of zwitterionic selfâ€assembled monolayers. AICHE Journal, 2021, 67, e17103.	1.8	14
106	Homoporous polymer membrane via forced surface segregation: A computer simulation study. Chemical Engineering Science, 2018, 191, 490-499.	1.9	13
107	Enzymatic characterization of a recombinant carbonyl reductase from Acetobacter sp. CCTCC M209061. Bioresources and Bioprocessing, 2017, 4, 39.	2.0	12
108	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.	4.1	12

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109	Computer simulations on double hydrophobic PS-b-PMMA porous membrane by non-solvent induced phase separation. Fluid Phase Equilibria, 2020, 523, 112784.	1.4	12
110	The application of poly(methyl methacrylate-co-butyl acrylate-co-styrene) in reinforcing fragile papers: experiments and computer simulations. Cellulose, 2017, 24, 5157-5171.	2.4	11
111	Molecular simulations of charged complex fluids: A review. Chinese Journal of Chemical Engineering, 2021, 31, 206-226.	1.7	11
112	Two-dimensional self-assembly of esters with different configurations at the liquidâ€“solid interface. Applied Surface Science, 2011, 257, 4559-4565.	3.1	10
113	Simulation Insight into the Synergic Role of Citrate and Polyaspartic Peptide in Biomineralization. Langmuir, 2021, 37, 3410-3419.	1.6	10
114	Computer simulation of zwitterionic polymer brush grafted silica nanoparticles to modify polyvinylidene fluoride membrane. Journal of Colloid and Interface Science, 2021, 587, 173-182.	5.0	10
115	Simulated preparation and hydration property of a new-generation zwitterionic modified PVDF membrane. Journal of Membrane Science, 2022, 652, 120498.	4.1	10
116	Orientation and Conformation of Hydrophobin at the Oilâ€“Water Interface: Insights from Molecular Dynamics Simulations. Langmuir, 2022, 38, 6191-6200.	1.6	9
117	Lysozyme Adsorption on Porous Organic Cages: A Molecular Simulation Study. Langmuir, 2020, 36, 12299-12308.	1.6	8
118	Lysozyme Adsorption on Different Functionalized MXenes: A Multiscale Simulation Study. Langmuir, 2021, 37, 5932-5942.	1.6	6
119	A coarse-grained simulation of heat and mass transfer through a graphene oxide-based composite membrane. Chemical Engineering Science, 2021, 243, 116692.	1.9	6
120	Molecular understanding of acetylcholinesterase adsorption on functionalized carbon nanotubes for enzymatic biosensors. Physical Chemistry Chemical Physics, 2022, 24, 2866-2878.	1.3	6
121	Dual-responsive zwitterion-modified nanopores: a mesoscopic simulation study. Journal of Materials Chemistry B, 2022, 10, 2740-2749.	2.9	6
122	Modulating the Adsorption Orientation of Methionine-rich Laccase by Tailoring the Surface Chemistry of Single-walled Carbon Nanotubes. Colloids and Surfaces B: Biointerfaces, 2022, , 112660.	2.5	5
123	Molecular Thin Films on Solid Surfaces: Mechanisms of Melting. Langmuir, 2012, 28, 7382-7392.	1.6	4
124	Effect of Topology of Hydrophobic Surfaces on Their Wetting States by Coarse-grained Simulations. Acta Chimica Sinica, 2014, 72, 1075.	0.5	4
125	The interplay between surface-functionalized gold nanoparticles and negatively charged lipid vesicles. Physical Chemistry Chemical Physics, 2021, 23, 23526-23536.	1.3	4
126	Mesoscopic Structure of Nafion-Ionic Liquid Membrane Using Dissipative Particle Dynamics Simulations. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2016, 32, 1649-1657.	2.2	3

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127	Computer simulations of underwater oil adhesion of self-assembled monolayers on Au (111). Molecular Simulation, 2020, 46, 713-720.	0.9	3
128	Replica Exchange Molecular Dynamics Simulations on the Folding of Trpzip4 Î²-Hairpin. Acta Chimica Sinica, 2013, 71, 593.	0.5	3
129	ACAP1 assembles into an unusual protein lattice for membrane deformation through multiple stages. PLoS Computational Biology, 2019, 15, e1007081.	1.5	2
130	Crystallization of Sodium Bicarbonate in the Presence of Trace Amounts of HPMA. ChemistrySelect, 2021, 6, 2184-2188.	0.7	2
131	Computer Simulations of Fibronectin Adsorption on Graphene Modified Titanium Dioxide Surfaces. Acta Chimica Sinica, 2014, 72, 401.	0.5	2
132	Surface Structure and Interaction of Surface/Interface Probed by Mesoscale Simulations and Experiments. Advances in Chemical Engineering, 2015, 47, 85-162.	0.5	1
133	Simulated synthesis of silica nanowires by lyotropic liquid crystal template method. Molecular Simulation, 0, , 1-11.	0.9	0