

Jia-Wei Shen

List of Publications by Year in descending order

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70
papers

2,141
citations

236612

25
h-index

243296

44
g-index

70
all docs

70
docs citations

70
times ranked

2624
citing authors

#	ARTICLE	IF	CITATIONS
1	Understanding the anchoring interaction of coagulation factor Va light chain on zeolites: A molecular dynamics study. <i>Journal of Colloid and Interface Science</i> , 2022, 608, 435-445.	5.0	3
2	Pore size control of monodisperse mesoporous silica particles with alkyl imidazole ionic liquid templates for high performance liquid chromatography applications. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 637, 128200.	2.3	5
3	Dynamics of electric field-controlled methotrexate delivery through membrane nanochannels. <i>Journal of Molecular Liquids</i> , 2022, 350, 118525.	2.3	0
4	Design lamellar GO membrane based on understanding the effect of functional groups distributed in the pore on desalination. <i>Journal of Molecular Liquids</i> , 2022, 360, 119542.	2.3	4
5	A review on the cytotoxicity of graphene quantum dots: from experiment to simulation. <i>Nanoscale Advances</i> , 2021, 3, 904-917.	2.2	34
6	Effect of Shape on the Entering of Graphene Quantum Dots into a Membrane: A Molecular Dynamics Simulation. <i>ACS Omega</i> , 2021, 6, 10936-10943.	1.6	17
7	Molecular insights into desalination performance of lamellar graphene membranes: Significant of hydrophobicity and interlayer spacing. <i>Journal of Molecular Liquids</i> , 2021, 333, 116024.	2.3	21
8	Enantioseparation of cloprostenol on the polysaccharide chiral stationary phase: Influence of the mobile phase on enantioselective adsorption. <i>Journal of Chromatography A</i> , 2021, 1653, 462413.	1.8	3
9	Direct proof of soft knock-on mechanism of ion permeation in a voltage gated sodium channel. <i>International Journal of Biological Macromolecules</i> , 2021, 188, 369-374.	3.6	1
10	Theoretical investigation on the adsorption orientation of DNA on two-dimensional MoSe ₂ . <i>Chemical Physics</i> , 2021, 551, 111329.	0.9	2
11	A review on desalination by graphene-based biomimetic nanopore: From the computational modelling perspective. <i>Journal of Molecular Liquids</i> , 2021, 342, 117582.	2.3	12
12	Study on the adsorption orientation of DNA on two-dimensional MoS ₂ surface via molecular dynamics simulation: A vertical orientation phenomenon. <i>Chemical Physics</i> , 2020, 529, 110546.	0.9	14
13	A molecular dynamics study on water desalination using single-layer MoSe ₂ nanopore. <i>Journal of Membrane Science</i> , 2020, 595, 117611.	4.1	40
14	DNA fragment translocation through the lipid membrane assisted by carbon nanotube. <i>International Journal of Pharmaceutics</i> , 2020, 574, 118921.	2.6	8
15	A subtraction fitting method for independent determination of enantioselective and nonselective adsorption isotherms based on the single-component isotherms in the framework of the two-site model. <i>Journal of Chromatography A</i> , 2020, 1632, 461608.	1.8	2
16	Characterization of water structure in carbon nanotubes by various order parameters. <i>Chemical Physics</i> , 2020, 538, 110887.	0.9	1
17	Molecular dynamics study on the adsorption and release of doxorubicin by chitosan-decorated graphene. <i>Carbohydrate Polymers</i> , 2020, 248, 116809.	5.1	20
18	Theoretical Evaluation of DNA Genotoxicity of Graphene Quantum Dots: A Combination of Density Functional Theory and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9335-9342.	1.2	26

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19	On the mechanism of graphene quantum dot encapsulation by chitosan: A molecular dynamics study. <i>Journal of Molecular Liquids</i> , 2020, 320, 113453.	2.3	7
20	Monodisperse core-shell silica particles as a high-performance liquid chromatography packing material: Facile in situ silica sol-gel synthesis. <i>Journal of Chromatography A</i> , 2020, 1625, 461282.	1.8	7
21	Novel chiral stationary phases based on 3,5-dimethyl phenylcarbamoylated β -cyclodextrin combining cinchona alkaloid moiety. <i>Chirality</i> , 2020, 32, 1080-1090.	1.3	6
22	Understanding the effect of hydroxyl/epoxy group on water desalination through lamellar graphene oxide membranes via molecular dynamics simulation. <i>Desalination</i> , 2020, 491, 114560.	4.0	47
23	Molecular dynamics study on the encapsulation and release of anti-cancer drug doxorubicin by chitosan. <i>International Journal of Pharmaceutics</i> , 2020, 580, 119241.	2.6	41
24	Atomistic insights into the separation mechanism of multilayer graphene membranes for water desalination. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7224-7233.	1.3	27
25	Understanding the effect of chemical modification on water desalination in boron nitride nanotubes via molecular dynamics simulation. <i>Desalination</i> , 2019, 464, 84-93.	4.0	45
26	Graphene quantum dot assisted translocation of drugs into a cell membrane. <i>Nanoscale</i> , 2019, 11, 4503-4514.	2.8	56
27	Understanding the size effect of graphene quantum dots on protein adsorption. <i>Colloids and Surfaces B: Biointerfaces</i> , 2019, 174, 575-581.	2.5	24
28	Charge-tunable water transport through boron nitride nanotubes. <i>Journal of Molecular Liquids</i> , 2018, 258, 98-105.	2.3	16
29	Molecular dynamics study on the configuration and arrangement of doxorubicin in carbon nanotubes. <i>Journal of Molecular Liquids</i> , 2018, 262, 295-301.	2.3	35
30	Theoretical studies on key factors in DNA sequencing using atomically thin molybdenum disulfide nanopores. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28886-28893.	1.3	7
31	DNA sequencing by two-dimensional materials: As theoretical modeling meets experiments. <i>Biosensors and Bioelectronics</i> , 2017, 89, 280-292.	5.3	35
32	Molecular dynamics study on DNA nanotubes as drug delivery vehicle for anticancer drugs. <i>Colloids and Surfaces B: Biointerfaces</i> , 2017, 153, 168-173.	2.5	44
33	Theoretical study on the interaction of nucleotides on two-dimensional atomically thin graphene and molybdenum disulfide. <i>FlatChem</i> , 2017, 2, 8-14.	2.8	23
34	Investigation of the morphological transition of a phospholipid bilayer membrane in an external electric field via molecular dynamics simulation. <i>Journal of Molecular Modeling</i> , 2017, 23, 113.	0.8	6
35	Computer simulation of water desalination through boron nitride nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30031-30038.	1.3	28
36	Pressing Carbon Nanotubes Triggers Better Ion Selectivity. <i>Journal of Physical Chemistry C</i> , 2017, 121, 19512-19518.	1.5	3

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37	Molecular dynamics study on the mechanism of polynucleotide encapsulation by chitosan. <i>Scientific Reports</i> , 2017, 7, 5050.	1.6	32
38	Adsorption Behavior and Mechanism of SCA-1 on a Calcite Surface: A Molecular Dynamics Study. <i>Langmuir</i> , 2017, 33, 11321-11331.	1.6	11
39	A Novel Derivative of (-)-mycosanine Produced by the Endophytic Fungus <i>Mycosphaerella nawae</i> , Exhibits High and Selective Immunosuppressive Activity on T Cells. <i>Frontiers in Microbiology</i> , 2017, 8, 1251.	1.5	26
40	Plasma Fibulin-3 as a Potential Biomarker for Patients with Asbestos-Related Diseases in the Han Population. <i>Disease Markers</i> , 2017, 2017, 1-8.	0.6	14
41	Theoretic Study on Dispersion Mechanism of Boron Nitride Nanotubes by Polynucleotides. <i>Scientific Reports</i> , 2016, 6, 39747.	1.6	10
42	Controlled interval of aligned carbon nanotubes arrays for water desalination: A molecular dynamics simulation study. <i>Desalination</i> , 2016, 395, 28-32.	4.0	22
43	Molecular modelling of translocation of biomolecules in carbon nanotubes: method, mechanism and application. <i>Molecular Simulation</i> , 2016, 42, 827-835.	0.9	17
44	The effect of spacer on the structure of surfactant at liquid/air interface: A molecular dynamics simulation study. <i>Journal of Molecular Liquids</i> , 2016, 222, 988-994.	2.3	4
45	The self-assembly mechanism of tetra-peptides from the motif of β -amyloid peptides: a combined coarse-grained and all-atom molecular dynamics simulation. <i>RSC Advances</i> , 2016, 6, 100072-100078.	1.7	10
46	Theoretical Evaluation on Potential Cytotoxicity of Graphene Quantum Dots. <i>ACS Biomaterials Science and Engineering</i> , 2016, 2, 1983-1991.	2.6	65
47	Translocation mechanism of C60 and C60 derivations across a cell membrane. <i>Journal of Nanoparticle Research</i> , 2016, 18, 1.	0.8	8
48	Charge-tunable insertion process of carbon nanotubes into DNA nanotubes. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 66, 20-25.	1.3	12
49	Charge-tunable absorption behavior of DNA on graphene. <i>Journal of Materials Chemistry B</i> , 2015, 3, 4814-4820.	2.9	23
50	On the loading mechanism of ssDNA into carbon nanotubes. <i>RSC Advances</i> , 2015, 5, 56896-56903.	1.7	15
51	Molecular dynamics simulations indicate that DNA bases using graphene nanopores can be identified by their translocation times. <i>RSC Advances</i> , 2015, 5, 9389-9395.	1.7	12
52	Understanding the Structure of Hydrophobic Surfactants at the Air/Water Interface from Molecular Level. <i>Langmuir</i> , 2014, 30, 13815-13822.	1.6	23
53	Theoretical studies on the dynamics of DNA fragment translocation through multilayer graphene nanopores. <i>RSC Advances</i> , 2014, 4, 50494-50502.	1.7	17
54	Effects of Graphene Nanopore Geometry on DNA Sequencing. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1602-1607.	2.1	54

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55	Molecular dynamics study on the interaction between doxorubicin and hydrophobically modified chitosan oligosaccharide. RSC Advances, 2014, 4, 23730-23739.	1.7	29
56	Understanding the Control of Mineralization by Polyelectrolyte Additives: Simulation of Preferential Binding to Calcite Surfaces. Journal of Physical Chemistry C, 2013, 117, 6904-6913.	1.5	57
57	A Chemically Accurate Implicit-Solvent Coarse-Grained Model for Polystyrenesulfonate Solutions. Macromolecules, 2012, 45, 2551-2561.	2.2	38
58	Transferability of Coarse Grained Potentials: Implicit Solvent Models for Hydrated Ions. Journal of Chemical Theory and Computation, 2011, 7, 1916-1927.	2.3	52
59	Diameter Selectivity of Protein Encapsulation in Carbon Nanotubes. Journal of Physical Chemistry B, 2010, 114, 2869-2875.	1.2	37
60	Adsorption of Insulin Peptide on Charged Single-Walled Carbon Nanotubes: Significant Role of Ordered Water Molecules. ChemPhysChem, 2009, 10, 1260-1269.	1.0	22
61	On the spontaneous encapsulation of proteins in carbon nanotubes. Biomaterials, 2009, 30, 2807-2815.	5.7	110
62	Molecular Dynamics Simulation on Stability of Insulin on Graphene. Chinese Journal of Chemical Physics, 2009, 22, 627-634.	0.6	25
63	Molecular simulation of protein adsorption and desorption on hydroxyapatite surfaces. Biomaterials, 2008, 29, 513-532.	5.7	249
64	Induced stepwise conformational change of human serum albumin on carbon nanotube surfaces. Biomaterials, 2008, 29, 3847-3855.	5.7	141
65	Shield effect of silicate on adsorption of proteins onto silicon-doped hydroxyapatite (100) surface. Biomaterials, 2008, 29, 2423-2432.	5.7	66
66	Diffusion dynamics of water controlled by topology of potential energy surface inside carbon nanotubes. Physical Review B, 2008, 77, .	1.1	59
67	Conformational Mobility of GOx Coenzyme Complex on Single-Wall Carbon Nanotubes. Sensors, 2008, 8, 8453-8462.	2.1	16
68	Adsorption mechanism of BMP-7 on hydroxyapatite (001) surfaces. Biochemical and Biophysical Research Communications, 2007, 361, 91-96.	1.0	106
69	Adsorption of Leucine-Rich Amelogenin Protein on Hydroxyapatite (001) Surface through α -COO-Claws. Journal of Physical Chemistry C, 2007, 111, 1284-1290.	1.5	85
70	Theoretical investigation on the mechanism of phospholipid extraction from the cell membrane using functionalized graphene quantum dots. Materials Advances, 0, , .	2.6	4