Jia-Wei Shen

List of Publications by Year
in descending order

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70	2,141	236925	243625
papers	citations	25 h-index	44 g-index

70	70	70	2624
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Understanding the anchoring interaction of coagulation factor Va light chain on zeolites: A molecular dynamics study. Journal of Colloid and Interface Science, 2022, 608, 435-445.	9.4	3
2	Pore size control of monodisperse mesoporous silica particles with alkyl imidazole ionic liquid templates for high performance liquid chromatography applications. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 637, 128200.	4.7	5
3	Dynamics of electric field-controlled methotrexate delivery through membrane nanochannels. Journal of Molecular Liquids, 2022, 350, 118525.	4.9	0
4	Design lamellar GO membrane based on understanding the effect of functional groups distributed in the port on desalination. Journal of Molecular Liquids, 2022, 360, 119542.	4.9	4
5	A review on the cytotoxicity of graphene quantum dots: from experiment to simulation. Nanoscale Advances, 2021, 3, 904-917.	4.6	34
6	Effect of Shape on the Entering of Graphene Quantum Dots into a Membrane: A Molecular Dynamics Simulation. ACS Omega, 2021, 6, 10936-10943.	3.5	17
7	Molecular insights into desalination performance of lamellar graphene membranes: Significant of hydrophobicity and interlayer spacing. Journal of Molecular Liquids, 2021, 333, 116024.	4.9	21
8	Enantioseparation of cloprostenol on the polysaccharide chiral stationary phase: Influence of the mobile phase on enantioselective adsorption. Journal of Chromatography A, 2021, 1653, 462413.	3.7	3
9	Direct proof of soft knock-on mechanism of ion permeation in a voltage gated sodium channel. International Journal of Biological Macromolecules, 2021, 188, 369-374.	7.5	1
10	Theoretical investigation on the adsorption orientation of DNA on two-dimensional MoSe2. Chemical Physics, 2021, 551, 111329.	1.9	2
11	A review on desalination by graphene-based biomimetic nanopore: From the computational modelling perspective. Journal of Molecular Liquids, 2021, 342, 117582.	4.9	12
12	Study on the adsorption orientation of DNA on two-dimensional MoS2 surface via molecular dynamics simulation: A vertical orientation phenomenon. Chemical Physics, 2020, 529, 110546.	1.9	14
13	A molecular dynamics study on water desalination using single-layer MoSe2 nanopore. Journal of Membrane Science, 2020, 595, 117611.	8.2	40
14	DNA fragment translocation through the lipid membrane assisted by carbon nanotube. International Journal of Pharmaceutics, 2020, 574, 118921.	5.2	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. Journal of Chromatography A, 2020, 1632, 461608.	3.7	2
16	Characterization of water structure in carbon nanotubes by various order parameters. Chemical Physics, 2020, 538, 110887.	1.9	1
17	Molecular dynamics study on the adsorption and release of doxorubicin by chitosan-decorated graphene. Carbohydrate Polymers, 2020, 248, 116809.	10.2	20
18	Theoretical Evaluation of DNA Genotoxicity of Graphene Quantum Dots: A Combination of Density Functional Theory and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 9335-9342.	2.6	26

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19	On the mechanism of graphene quantum dot encapsulation by chitosan: A molecular dynamics study. Journal of Molecular Liquids, 2020, 320, 113453.	4.9	7
20	Monodisperse coreâ€“shell silica particles as a high-performance liquid chromatography packing material: Facile in situ silica sol-gel synthesis. Journal of Chromatography A, 2020, 1625, 461282.	3.7	7
21	Novel chiral stationary phases based on 3,5â€dimethyl phenylcarbamoylated Î²â€cyclodextrin combining cinchona alkaloid moiety. Chirality, 2020, 32, 1080-1090.	2.6	6
22	Understanding the effect of hydroxyl/epoxy group on water desalination through lamellar graphene oxide membranes via molecular dynamics simulation. Desalination, 2020, 491, 114560.	8.2	47
23	Molecular dynamics study on the encapsulation and release of anti-cancer drug doxorubicin by chitosan. International Journal of Pharmaceutics, 2020, 580, 119241.	5.2	41
24	Atomistic insights into the separation mechanism of multilayer graphene membranes for water desalination. Physical Chemistry Chemical Physics, 2020, 22, 7224-7233.	2.8	27
25	Understanding the effect of chemical modification on water desalination in boron nitride nanotubes via molecular dynamics simulation. Desalination, 2019, 464, 84-93.	8.2	45
26	Graphene quantum dot assisted translocation of drugs into a cell membrane. Nanoscale, 2019, 11, 4503-4514.	5.6	56
27	Understanding the size effect of graphene quantum dots on protein adsorption. Colloids and Surfaces B: Biointerfaces, 2019, 174, 575-581.	5.0	24
28	Charge-tunable water transport through boron nitride nanotubes. Journal of Molecular Liquids, 2018, 258, 98-105.	4.9	16
29	Molecular dynamics study on the configuration and arrangement of doxorubicin in carbon nanotubes. Journal of Molecular Liquids, 2018, 262, 295-301.	4.9	35
30	Theoretical studies on key factors in DNA sequencing using atomically thin molybdenum disulfide nanopores. Physical Chemistry Chemical Physics, 2018, 20, 28886-28893.	2.8	7
31	DNA sequencing by two-dimensional materials: As theoretical modeling meets experiments. Biosensors and Bioelectronics, 2017, 89, 280-292.	10.1	35
32	Molecular dynamics study on DNA nanotubes as drug delivery vehicle for anticancer drugs. Colloids and Surfaces B: Biointerfaces, 2017, 153, 168-173.	5.0	44
33	Theoretical study on the interaction of nucleotides on two-dimensional atomically thin graphene and molybdenum disulfide. FlatChem, 2017, 2, 8-14.	5.6	23
34	Investigation of the morphological transition of a phospholipid bilayer membrane in an external electric field via molecular dynamics simulation. Journal of Molecular Modeling, 2017, 23, 113.	1.8	6
35	Computer simulation of water desalination through boron nitride nanotubes. Physical Chemistry Chemical Physics, 2017, 19, 30031-30038.	2.8	28
36	Pressing Carbon Nanotubes Triggers Better Ion Selectivity. Journal of Physical Chemistry C, 2017, 121, 19512-19518.	3.1	3

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37	Molecular dynamics study on the mechanism of polynucleotide encapsulation by chitosan. Scientific Reports, 2017, 7, 5050.	3.3	32
38	Adsorption Behavior and Mechanism of SCA-1 on a Calcite Surface: A Molecular Dynamics Study. Langmuir, 2017, 33, 11321-11331.	3.5	11
39	A Novel Derivative of (-)mycousnine Produced by the Endophytic Fungus Mycosphaerella nawae, Exhibits High and Selective Immunosuppressive Activity on T Cells. Frontiers in Microbiology, 2017, 8, 1251.	3.5	26
40	Plasma Fibulin-3 as a Potential Biomarker for Patients with Asbestos-Related Diseases in the Han Population. Disease Markers, 2017, 2017, 1-8.	1.3	14
41	Theoretic Study on Dispersion Mechanism of Boron Nitride Nanotubes by Polynucleotides. Scientific Reports, 2016, 6, 39747.	3.3	10
42	Controlled interval of aligned carbon nanotubes arrays for water desalination: A molecular dynamics simulation study. Desalination, 2016, 395, 28-32.	8.2	22
43	Molecular modelling of translocation of biomolecules in carbon nanotubes: method, mechanism and application. Molecular Simulation, 2016, 42, 827-835.	2.0	17
44	The effect of spacer on the structure of surfactant at liquid/air interface: A molecular dynamics simulation study. Journal of Molecular Liquids, 2016, 222, 988-994.	4.9	4
45	The self-assembly mechanism of tetra-peptides from the motif of Î²-amyloid peptides: a combined coarse-grained and all-atom molecular dynamics simulation. RSC Advances, 2016, 6, 100072-100078.	3.6	10
46	Theoretical Evaluation on Potential Cytotoxicity of Graphene Quantum Dots. ACS Biomaterials Science and Engineering, 2016, 2, 1983-1991.	5.2	65
47	Translocation mechanism of C60 and C60 derivations across a cell membrane. Journal of Nanoparticle Research, 2016, 18, 1.	1.9	8
48	Charge-tunable insertion process of carbon nanotubes into DNA nanotubes. Journal of Molecular Graphics and Modelling, 2016, 66, 20-25.	2.4	12
49	Charge-tunable absorption behavior of DNA on graphene. Journal of Materials Chemistry B, 2015, 3, 4814-4820.	5.8	23
50	On the loading mechanism of ssDNA into carbon nanotubes. RSC Advances, 2015, 5, 56896-56903.	3.6	15
51	Molecular dynamics simulations indicate that DNA bases using graphene nanopores can be identified by their translocation times. RSC Advances, 2015, 5, 9389-9395.	3.6	12
52	Understanding the Structure of Hydrophobic Surfactants at the Air/Water Interface from Molecular Level. Langmuir, 2014, 30, 13815-13822.	3.5	23
53	Theoretical studies on the dynamics of DNA fragment translocation through multilayer graphene nanopores. RSC Advances, 2014, 4, 50494-50502.	3.6	17
54	Effects of Graphene Nanopore Geometry on DNA Sequencing. Journal of Physical Chemistry Letters, 2014, 5, 1602-1607.	4.6	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.	3.6	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.	3.1	57
57	A Chemically Accurate Implicit-Solvent Coarse-Grained Model for Polystyrenesulfonate Solutions. Macromolecules, 2012, 45, 2551-2561.	4.8	38
58	Transferability of Coarse Grained Potentials: Implicit Solvent Models for Hydrated Ions. Journal of Chemical Theory and Computation, 2011, 7, 1916-1927.	5.3	52
59	Diameter Selectivity of Protein Encapsulation in Carbon Nanotubes. Journal of Physical Chemistry B, 2010, 114, 2869-2875.	2.6	37
60	Adsorption of Insulin Peptide on Charged Singleâ€Walled Carbon Nanotubes: Significant Role of Ordered Water Molecules. ChemPhysChem, 2009, 10, 1260-1269.	2.1	22
61	On the spontaneous encapsulation of proteins in carbon nanotubes. Biomaterials, 2009, 30, 2807-2815.	11.4	110
62	Molecular Dynamics Simulation on Stability of Insulin on Graphene. Chinese Journal of Chemical Physics, 2009, 22, 627-634.	1.3	25
63	Molecular simulation of protein adsorption and desorption on hydroxyapatite surfaces. Biomaterials, 2008, 29, 513-532.	11.4	249
64	Induced stepwise conformational change of human serum albumin on carbon nanotube surfaces. Biomaterials, 2008, 29, 3847-3855.	11.4	141
65	Shield effect of silicate on adsorption of proteins onto silicon-doped hydroxyapatite (100) surface. Biomaterials, 2008, 29, 2423-2432.	11.4	66
66	Diffusion dynamics of water controlled by topology of potential energy surface inside carbon nanotubes. Physical Review B, 2008, 77, .	3.2	59
67	Conformational Mobility of GOx Coenzyme Complex on Single-Wall Carbon Nanotubes. Sensors, 2008, 8, 8453-8462.	3.8	16
68	Adsorption mechanism of BMP-7 on hydroxyapatite (001) surfaces. Biochemical and Biophysical Research Communications, 2007, 361, 91-96.	2.1	106
69	Adsorption of Leucine-Rich Amelogenin Protein on Hydroxyapatite (001) Surface through â˜COO- Claws. Journal of Physical Chemistry C, 2007, 111, 1284-1290.	3.1	85
70	Theoretical investigation on the mechanism of phospholipid extraction from the cell membrane using functionalized graphene quantum dots. Materials Advances, 0, , .	5.4	4