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	Molecular simulation of protein adsorption and desorption on hydroxyapatite surfaces. Biomaterials, 2008, 29, 513-532.	11.4	249
2	Induced stepwise conformational change of human serum albumin on carbon nanotube surfaces. Biomaterials, 2008, 29, 3847-3855.	11.4	141
3	On the spontaneous encapsulation of proteins in carbon nanotubes. Biomaterials, 2009, 30, 2807-2815.	11.4	110
4	Adsorption mechanism of BMP-7 on hydroxyapatite (001) surfaces. Biochemical and Biophysical Research Communications, 2007, 361, 91-96.	2.1	106
5	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
6	Shield effect of silicate on adsorption of proteins onto silicon-doped hydroxyapatite (100) surface. Biomaterials, 2008, 29, 2423-2432.	11.4	66
7	Theoretical Evaluation on Potential Cytotoxicity of Graphene Quantum Dots. ACS Biomaterials Science and Engineering, 2016, 2, 1983-1991.	5.2	65
8	Diffusion dynamics of water controlled by topology of potential energy surface inside carbon nanotubes. Physical Review B, 2008, 77, .	3.2	59
9	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
10	Graphene quantum dot assisted translocation of drugs into a cell membrane. Nanoscale, 2019, 11, 4503-4514.	5.6	56
11	Effects of Graphene Nanopore Geometry on DNA Sequencing. Journal of Physical Chemistry Letters, 2014, 5, 1602-1607.	4.6	54
12	Transferability of Coarse Grained Potentials: Implicit Solvent Models for Hydrated Ions. Journal of Chemical Theory and Computation, 2011, 7, 1916-1927.	5.3	52
13	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
14	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
15	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
16	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
17	A molecular dynamics study on water desalination using single-layer MoSe2 nanopore. Journal of Membrane Science, 2020, 595, 117611.	8.2	40
18	A Chemically Accurate Implicit-Solvent Coarse-Grained Model for Polystyrenesulfonate Solutions. Macromolecules, 2012, 45, 2551-2561.	4.8	38

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19	Diameter Selectivity of Protein Encapsulation in Carbon Nanotubes. Journal of Physical Chemistry B, 2010, 114, 2869-2875.	2.6	37
20	DNA sequencing by two-dimensional materials: As theoretical modeling meets experiments. Biosensors and Bioelectronics, 2017, 89, 280-292.	10.1	35
21	Molecular dynamics study on the configuration and arrangement of doxorubicin in carbon nanotubes. Journal of Molecular Liquids, 2018, 262, 295-301.	4.9	35
22	A review on the cytotoxicity of graphene quantum dots: from experiment to simulation. Nanoscale Advances, 2021, 3, 904-917.	4.6	34
23	Molecular dynamics study on the mechanism of polynucleotide encapsulation by chitosan. Scientific Reports, 2017, 7, 5050.	3.3	32
24	Molecular dynamics study on the interaction between doxorubicin and hydrophobically modified chitosan oligosaccharide. RSC Advances, 2014, 4, 23730-23739.	3.6	29
25	Computer simulation of water desalination through boron nitride nanotubes. Physical Chemistry Chemical Physics, 2017, 19, 30031-30038.	2.8	28
26	Atomistic insights into the separation mechanism of multilayer graphene membranes for water desalination. Physical Chemistry Chemical Physics, 2020, 22, 7224-7233.	2.8	27
27	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
28	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
29	Molecular Dynamics Simulation on Stability of Insulin on Graphene. Chinese Journal of Chemical Physics, 2009, 22, 627-634.	1.3	25
30	Understanding the size effect of graphene quantum dots on protein adsorption. Colloids and Surfaces B: Biointerfaces, 2019, 174, 575-581.	5.0	24
31	Understanding the Structure of Hydrophobic Surfactants at the Air/Water Interface from Molecular Level. Langmuir, 2014, 30, 13815-13822.	3.5	23
32	Charge-tunable absorption behavior of DNA on graphene. Journal of Materials Chemistry B, 2015, 3, 4814-4820.	5.8	23
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	Adsorption of Insulin Peptide on Charged Singleâ€Walled Carbon Nanotubes: Significant Role of Ordered Water Molecules. ChemPhysChem, 2009, 10, 1260-1269.	2.1	22
35	Controlled interval of aligned carbon nanotubes arrays for water desalination: A molecular dynamics simulation study. Desalination, 2016, 395, 28-32.	8.2	22
36	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

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37	Molecular dynamics study on the adsorption and release of doxorubicin by chitosan-decorated graphene. Carbohydrate Polymers, 2020, 248, 116809.	10.2	20
38	Theoretical studies on the dynamics of DNA fragment translocation through multilayer graphene nanopores. RSC Advances, 2014, 4, 50494-50502.	3.6	17
39	Molecular modelling of translocation of biomolecules in carbon nanotubes: method, mechanism and application. Molecular Simulation, 2016, 42, 827-835.	2.0	17
40	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
41	Conformational Mobility of GOx Coenzyme Complex on Single-Wall Carbon Nanotubes. Sensors, 2008, 8, 8453-8462.	3.8	16
42	Charge-tunable water transport through boron nitride nanotubes. Journal of Molecular Liquids, 2018, 258, 98-105.	4.9	16
43	On the loading mechanism of ssDNA into carbon nanotubes. RSC Advances, 2015, 5, 56896-56903.	3.6	15
44	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
45	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
46	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
47	Charge-tunable insertion process of carbon nanotubes into DNA nanotubes. Journal of Molecular Graphics and Modelling, 2016, 66, 20-25.	2.4	12
48	A review on desalination by graphene-based biomimetic nanopore: From the computational modelling perspective. Journal of Molecular Liquids, 2021, 342, 117582.	4.9	12
49	Adsorption Behavior and Mechanism of SCA-1 on a Calcite Surface: A Molecular Dynamics Study. Langmuir, 2017, 33, 11321-11331.	3.5	11
50	Theoretic Study on Dispersion Mechanism of Boron Nitride Nanotubes by Polynucleotides. Scientific Reports, 2016, 6, 39747.	3.3	10
51	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
52	Translocation mechanism of C60 and C60 derivations across a cell membrane. Journal of Nanoparticle Research, 2016, 18, 1.	1.9	8
53	DNA fragment translocation through the lipid membrane assisted by carbon nanotube. International Journal of Pharmaceutics, 2020, 574, 118921.	5.2	8
54	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

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55	On the mechanism of graphene quantum dot encapsulation by chitosan: A molecular dynamics study. Journal of Molecular Liquids, 2020, 320, 113453.	4.9	7
56	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
57	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
58	Novel chiral stationary phases based on 3,5â€dimethyl phenylcarbamoylated Î²â€cyclodextrin combining cinchona alkaloid moiety. Chirality, 2020, 32, 1080-1090.	2.6	6
59	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
60	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
61	Theoretical investigation on the mechanism of phospholipid extraction from the cell membrane using functionalized graphene quantum dots. Materials Advances, 0, , .	5.4	4
62	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
63	Pressing Carbon Nanotubes Triggers Better Ion Selectivity. Journal of Physical Chemistry C, 2017, 121, 19512-19518.	3.1	3
64	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
65	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
66	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
67	Theoretical investigation on the adsorption orientation of DNA on two-dimensional MoSe2. Chemical Physics, 2021, 551, 111329.	1.9	2
68	Characterization of water structure in carbon nanotubes by various order parameters. Chemical Physics, 2020, 538, 110887.	1.9	1
69	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
70	Dynamics of electric field-controlled methotrexate delivery through membrane nanochannels. Journal of Molecular Liquids, 2022, 350, 118525.	4.9	0