Li-Jun Liang

List of Publications by Year
in descending order

71 papers	1,516 citations	279701 23 h-index	360920 35 g-index
71 all docs	71 docs citations	71 times ranked	1942 citing authors

#	Article	IF	Citations
1	Theoretical Investigation of Chitosan-Assisted Controlled Release of Digestive System Antitumor Drug Fluorouracil. Journal of Pharmaceutical Sciences, 2022, 111, 2049-2055.	1.6	1
2	Dynamics of electric field-controlled methotrexate delivery through membrane nanochannels. Journal of Molecular Liquids, 2022, 350, 118525.	2.3	0
3	Graphene-based woven filter membrane with excellent strength and efficiency for water desalination. Desalination, 2022, 533, 115775.	4.0	13
4	Pore Formation Mechanism of A-Beta Peptide on the Fluid Membrane: A Combined Coarse-Grained and All-Atomic Model. Molecules, 2022, 27, 3924.	1.7	1
5	A review on the cytotoxicity of graphene quantum dots: from experiment to simulation. Nanoscale Advances, 2021, 3, 904-917.	2.2	34
6	Simultaneous binding mechanism of multiple substrates for multidrug resistance transporter P-glycoprotein. Physical Chemistry Chemical Physics, 2021, 23, 4530-4543.	1.3	10
7	Effect of Shape on the Entering of Graphene Quantum Dots into a Membrane: A Molecular Dynamics Simulation. ACS Omega, 2021, 6, 10936-10943.	1.6	17
8	Molecular insights into desalination performance of lamellar graphene membranes: Significant of hydrophobicity and interlayer spacing. Journal of Molecular Liquids, 2021, 333, 116024.	2.3	21
9	A machine learning vibrational spectroscopy protocol for spectrum prediction and spectrum-based structure recognition. Fundamental Research, 2021, 1, 488-494.	1.6	19
10	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.	3.6	1
11	Theoretical investigation on the adsorption orientation of DNA on two-dimensional MoSe2. Chemical Physics, 2021, 551, 111329.	0.9	2
12	A review on desalination by graphene-based biomimetic nanopore: From the computational modelling perspective. Journal of Molecular Liquids, 2021, 342, 117582.	2.3	12
13	Release of an Encapsulated Peptide from Carbon Nanotubes Driven by Electric Fields: A Molecular Dynamics Study. ACS Omega, 2021, 6, 27485-27490.	1.6	4
14	Data-Driven Design of Nanopore Graphene for Water Desalination. Journal of Physical Chemistry C, 2021, 125, 27685-27692.	1.5	12
15	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.	0.9	14
16	A molecular dynamics study on water desalination using single-layer MoSe2 nanopore. Journal of Membrane Science, 2020, 595, 117611.	4.1	40
17	DNA fragment translocation through the lipid membrane assisted by carbon nanotube. International Journal of Pharmaceutics, 2020, 574, 118921.	2.6	8
18	Molecular dynamics study on loading mechanism of chitosan into boron nitride nanotubes. Journal of Molecular Liquids, 2020, 297, 111753.	2.3	7

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19	Characterization of water structure in carbon nanotubes by various order parameters. Chemical Physics, 2020, 538, 110887.	0.9	1
20	Molecular dynamics study on the adsorption and release of doxorubicin by chitosan-decorated graphene. Carbohydrate Polymers, 2020, 248, 116809.	5.1	20
21	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.	1.2	26
22	On the mechanism of graphene quantum dot encapsulation by chitosan: A molecular dynamics study. Journal of Molecular Liquids, 2020, 320, 113453.	2.3	7
23	Understanding the effect of hydroxyl/epoxy group on water desalination through lamellar graphene oxide membranes via molecular dynamics simulation. Desalination, 2020, 491, 114560.	4.0	47
24	Molecular dynamics study on the encapsulation and release of anti-cancer drug doxorubicin by chitosan. International Journal of Pharmaceutics, 2020, 580, 119241.	2.6	41
25	Atomistic insights into the separation mechanism of multilayer graphene membranes for water desalination. Physical Chemistry Chemical Physics, 2020, 22, 7224-7233.	1.3	27
26	On interactions of P-glycoprotein with various anti-tumor drugs by binding free energy calculations. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-13.	2.0	2
27	Versatile functionalization of surface-tailorable polymer nanohydrogels for drug delivery systems. Biomaterials Science, 2019, 7, 247-261.	2.6	10
28	Understanding the effect of chemical modification on water desalination in boron nitride nanotubes via molecular dynamics simulation. Desalination, 2019, 464, 84-93.	4.0	45
29	Graphene quantum dot assisted translocation of drugs into a cell membrane. Nanoscale, 2019, 11, 4503-4514.	2.8	56
30	Understanding the size effect of graphene quantum dots on protein adsorption. Colloids and Surfaces B: Biointerfaces, 2019, 174, 575-581.	2.5	24
31	Theoretical insights into aggregation-induced helicity modulation of a perylene bisimide derivative. Journal of Molecular Modeling, 2018, 24, 51.	0.8	4
32	Charge-tunable water transport through boron nitride nanotubes. Journal of Molecular Liquids, 2018, 258, 98-105.	2.3	16
33	Molecular dynamics study on the configuration and arrangement of doxorubicin in carbon nanotubes. Journal of Molecular Liquids, 2018, 262, 295-301.	2.3	35
34	Theoretical studies on key factors in DNA sequencing using atomically thin molybdenum disulfide nanopores. Physical Chemistry Chemical Physics, 2018, 20, 28886-28893.	1.3	7
35	Nanogel-Incorporated Injectable Hydrogel for Synergistic Therapy Based on Sequential Local Delivery of Combretastatin-A4 Phosphate (CA4P) and Doxorubicin (DOX). ACS Applied Materials & Interfaces, 2018, 10, 18560-18573.	4.0	82
36	DNA sequencing by two-dimensional materials: As theoretical modeling meets experiments. Biosensors and Bioelectronics, 2017, 89, 280-292.	5.3	35

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37	Molecular dynamics study on DNA nanotubes as drug delivery vehicle for anticancer drugs. Colloids and Surfaces B: Biointerfaces, 2017, 153, 168-173.	2.5	44
38	Theoretical study on the interaction of nucleotides on two-dimensional atomically thin graphene and molybdenum disulfide. FlatChem, 2017, 2, 8-14.	2.8	23
39	â€œClickâ€•functionalization of dual stimuli-responsive polymer nanocapsules for drug delivery systems. Polymer Chemistry, 2017, 8, 3056-3065.	1.9	28
40	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.	0.8	6
41	Computer simulation of water desalination through boron nitride nanotubes. Physical Chemistry Chemical Physics, 2017, 19, 30031-30038.	1.3	28
42	Pressing Carbon Nanotubes Triggers Better Ion Selectivity. Journal of Physical Chemistry C, 2017, 121, 19512-19518.	1.5	3
43	Molecular dynamics study on the mechanism of polynucleotide encapsulation by chitosan. Scientific Reports, 2017, 7, 5050.	1.6	32
44	Adsorption Behavior and Mechanism of SCA-1 on a Calcite Surface: A Molecular Dynamics Study. Langmuir, 2017, 33, 11321-11331.	1.6	11
45	Interaction between IGFBP7 and insulin: a theoretical and experimental study. Scientific Reports, 2016, 6, 19586.	1.6	10
46	Theoretic Study on Dispersion Mechanism of Boron Nitride Nanotubes by Polynucleotides. Scientific Reports, 2016, 6, 39747.	1.6	10
47	Controlled interval of aligned carbon nanotubes arrays for water desalination: A molecular dynamics simulation study. Desalination, 2016, 395, 28-32.	4.0	22
48	Molecular modelling of translocation of biomolecules in carbon nanotubes: method, mechanism and application. Molecular Simulation, 2016, 42, 827-835.	0.9	17
49	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.	1.7	10
50	Theoretical Evaluation on Potential Cytotoxicity of Graphene Quantum Dots. ACS Biomaterials Science and Engineering, 2016, 2, 1983-1991.	2.6	65
51	Translocation mechanism of C60 and C60 derivations across a cell membrane. Journal of Nanoparticle Research, 2016, 18, 1.	0.8	8
52	Insight into the adsorption profiles of the Saprolegnia monoica chitin synthase MIT domain on POPA and POPC membranes by molecular dynamics simulation studies. Physical Chemistry Chemical Physics, 2016, 18, 5281-5290.	1.3	11
53	Steered molecular dynamics study of inhibitor binding in the internal binding site in dehaloperoxidase-hemoglobin. Biophysical Chemistry, 2016, 211, 28-38.	1.5	20
54	Charge-tunable insertion process of carbon nanotubes into DNA nanotubes. Journal of Molecular Graphics and Modelling, 2016, 66, 20-25.	1.3	12

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55	Charge-tunable absorption behavior of DNA on graphene. Journal of Materials Chemistry B, 2015, 3, 4814-4820.	2.9	23
56	Interaction of P-glycoprotein with anti-tumor drugs: the site, gate and pathway. Soft Matter, 2015, 11, 6633-6641.	1.2	18
57	On the loading mechanism of ssDNA into carbon nanotubes. RSC Advances, 2015, 5, 56896-56903.	1.7	15
58	Molecular dynamics simulations indicate that DNA bases using graphene nanopores can be identified by their translocation times. RSC Advances, 2015, 5, 9389-9395.	1.7	12
59	Separation of Hydrogen Gas from Coal Gas by Graphene Nanopores. Journal of Physical Chemistry C, 2015, 119, 25559-25565.	1.5	42
60	Computational studies of DNA sequencing with solid-state nanopores: key issues and future prospects. Frontiers in Chemistry, 2014, 2, 5.	1.8	13
61	Peptide encapsulation regulated by the geometry of carbon nanotubes. Biomaterials, 2014, 35, 1771-1778.	5.7	19
62	Drug promiscuity of P-glycoprotein and its mechanism of interaction with paclitaxel and doxorubicin. Soft Matter, 2014, 10, 438-445.	1.2	36
63	Theoretical studies on the dynamics of DNA fragment translocation through multilayer graphene nanopores. RSC Advances, 2014, 4, 50494-50502.	1.7	17
64	A molecular dynamics study on pH response of protein adsorbed on peptide-modified polyvinyl alcohol hydrogel. Biomaterials Science, 2014, 2, 419-426.	2.6	23
65	Effects of Graphene Nanopore Geometry on DNA Sequencing. Journal of Physical Chemistry Letters, 2014, 5, 1602-1607.	2.1	54
66	Na⁺ and K⁺ ion selectivity by size-controlled biomimetic graphene nanopores. Nanoscale, 2014, 6, 10666-10672.	2.8	89
67	Contribution of Water Molecules in the Spontaneous Release of Protein by Graphene Sheets. ChemPhysChem, 2013, 14, 2902-2909.	1.0	6
68	Theoretical study on key factors in DNA sequencing with graphene nanopores. RSC Advances, 2013, 3, 2445.	1.7	41
69	Dispersion of Graphene Sheets in Aqueous Solution by Oligodeoxynucleotides. ChemPhysChem, 2013, 14, 1626-1632.	1.0	18
70	Molecular Dynamics Simulation on Stability of Insulin on Graphene. Chinese Journal of Chemical Physics, 2009, 22, 627-634.	0.6	25
71	Theoretical investigation on the mechanism of phospholipid extraction from the cell membrane using functionalized graphene quantum dots. Materials Advances, 0, , .	2.6	4