Jie Liu

List of Publications by Year in descending order

33 papers	985 citations	331538 21 h-index	434063 31 g-index
33 all docs	33 docs citations	33 times ranked	1122 citing authors

#	Article	IF	Citations
1	Machine Learning-Assisted Computational Screening of Metal-Organic Frameworks for Atmospheric Water Harvesting. Nanomaterials, 2022, 12, 159.	1.9	6
2	Porous Organic Cage Membranes for Biofuel Purification via Pervaporation: A Molecular Simulation Study. ACS Sustainable Chemistry and Engineering, 2021, 9, 14890-14899.	3.2	7
3	Machine learning and in silico discovery of metal-organic frameworks: Methanol as a working fluid in adsorption-driven heat pumps and chillers. Chemical Engineering Science, 2020, 214, 115430.	1.9	43
4	Porous organic cages as synthetic water channels. Nature Communications, 2020, 11, 4927.	5.8	43
5	Atomistic Simulation Study of Polyarylate/Zeolitic-Imidazolate Framework Mixed-Matrix Membranes for Water Desalination. ACS Applied Nano Materials, 2020, 3, 10022-10031.	2.4	23
6	Simulated revelation of the adsorption behaviours of acetylcholinesterase on charged self-assembled monolayers. Nanoscale, 2020, 12, 3701-3714.	2.8	25
7	Dipeptide membranes for CO2 separation: A molecular simulation study. Fluid Phase Equilibria, 2020, 515, 112570.	1.4	5
8	A Highly Rigid and Conjugated Microporous Polymer Membrane for Solvent Permeation and Biofuel Purification: A Molecular Simulation Study. ACS Sustainable Chemistry and Engineering, 2020, 8, 2892-2900.	3.2	14
9	Computational Screening of Metalâ€“Organic Framework Membranes for the Separation of 15 Gas Mixtures. Nanomaterials, 2019, 9, 467.	1.9	28
10	Microporous benzimidazole-linked polymer and its derivatives for organic solvent nanofiltration. Polymer, 2019, 185, 121932.	1.8	10
11	Combining large-scale screening and machine learning to predict the metal-organic frameworks for organosulfurs removal from high-sour natural gas. APL Materials, 2019, 7, .	2.2	22
12	An Atomistic Simulation Study on POC/PIM Mixed-Matrix Membranes for Gas Separation. Journal of Physical Chemistry C, 2019, 123, 15113-15121.	1.5	22
13	A molecular simulation study for efficient separation of 2,5-furandiyldimethanamine by a microporous polyarylate membrane. Polymer, 2019, 175, 8-14.	1.8	7
14	Molecular Design of Microporous Polymer Membranes for the Upgrading of Natural Gas. Journal of Physical Chemistry C, 2019, 123, 6607-6615.	1.5	17
15	A molecular simulation protocol for swelling and organic solvent nanofiltration of polymer membranes. Journal of Membrane Science, 2019, 573, 639-646.	4.1	50
16	Computational Design of 2D Covalent-Organic Framework Membranes for Organic Solvent Nanofiltration. ACS Sustainable Chemistry and Engineering, 2019, 7, 1734-1744.	3.2	52
17	A molecular simulation protocol for membrane pervaporation. Journal of Membrane Science, 2019, 572, 676-682.	4.1	22
18	Multiscale modeling and simulations of protein adsorption: progresses and perspectives. Current Opinion in Colloid and Interface Science, 2019, 41, 74-85.	3.4	65

#	Article	IF	Citations
19	Porous organic cages embedded in a lipid membrane for water desalination: A molecular simulation study. Journal of Membrane Science, 2019, 573, 177-183.	4.1	24
20	Zeolitic Imidazolate Framework Membranes for Organic Solvent Nanofiltration: A Molecular Simulation Exploration. ACS Applied Materials & Interfaces, 2018, 10, 33135-33143.	4.0	26
21	Solvent nanofiltration through polybenzimidazole membranes: Unravelling the role of pore size from molecular simulations. Journal of Membrane Science, 2018, 564, 782-787.	4.1	18
22	Bilirubin Oxidase Adsorption onto Charged Self-Assembled Monolayers: Insights from Multiscale Simulations. Langmuir, 2018, 34, 9818-9828.	1.6	32
23	Molecular Understanding of Laccase Adsorption on Charged Self-Assembled Monolayers. Journal of Physical Chemistry B, 2017, 121, 10610-10617.	1.2	29
24	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
25	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
26	Mesoscopic coarseâ€grained simulations of hydrophobic charge induction chromatography (HCIC) for protein purification. AIChE Journal, 2015, 61, 2035-2047.	1.8	35
27	Ribonuclease A adsorption onto charged self-assembled monolayers: A multiscale simulation study. Chemical Engineering Science, 2015, 121, 331-339.	1.9	45
28	Preparation and characterization of ZSM-5/PDMS hybrid pervaporation membranes: Laboratory results and pilot-scale performance. Separation and Purification Technology, 2015, 150, 257-267.	3.9	24
29	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
30	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
31	Mesoscopic Coarse-Grained Simulations of Lysozyme Adsorption. Journal of Physical Chemistry B, 2014, 118, 4451-4460.	1.2	66
32	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
33	Multiscale Simulations of Protein G B1 Adsorbed on Charged Self-Assembled Monolayers. Langmuir, 2013, 29, 11366-11374.	1.6	54