Jafar Azamat

List of Publications by Year in Descending Order

68 papers	907 citations	19 h-index	26 g-index
73 ext. papers	1,150 ext. citations	3.7 avg, IF	5.34 L-index

#	Paper	IF	Citations
68	Separation of CH4/N2 gas mixture using MFI zeolite nanosheet: Insights from molecular dynamics simulation. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2022**, 641, 128527	5.1	2
67	Molecular insight into water desalination through functionalized graphenylene nanosheet membranes. *Computational Materials Science*, **2022**, 203, 111126	3.2	2
66	Efficient water desalination through mono and bilayer carbon nitride nanosheet membranes: Insights from molecular dynamics simulation. *Journal of Molecular Graphics and Modelling*, **2022**, 110, 108059	2.8	3
65	The performance of a C2N membrane for heavy metal ions removal from water under external electric field. *Separation and Purification Technology*, **2022**, 289, 120770	8.3	0
64	A theoretical investigation into the effects of functionalized graphene nanosheets on dimethyl sulfoxide separation.. *Chemosphere*, **2022**, 134183	8.4	1
63	A new insight into the interaction of hydroxyl radical with supercooled nanodroplet in the atmosphere. *Journal of Molecular Liquids*, **2022**, 359, 119261	6	0
62	Efficient separation of He/CH mixture by functionalized graphenylene membranes: A theoretical study.. *Journal of Molecular Graphics and Modelling*, **2022**, 115, 108211	2.8	0
61	Efficient Removal of Heavy Metals from Aqueous Solutions through Functionalized Graphyne-1 Membranes under External Uniform Electric Fields: Insights from Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2021**, 125, 12254-12263	3.4	1
60	Molecular dynamics simulation of separation of water/methanol and water/ethanol mixture using boron nitride nanotubes. *Journal of Molecular Liquids*, **2021**, 331, 115774	6	4
59	Atomistic understanding of gas separation through nanoporous DDR-type zeolite membrane. *Chemical Physics*, **2021**, 540, 110985	2.3	5
58	Theoretical investigation of the removal of nitrate ions from contaminated aqueous solution using functionalized silicon carbide nanosheets. *Computational Materials Science*, **2021**, 187, 110118	3.2	5
57	Graphene Oxide and Reduced Graphene Oxide as Nanofillers in Membrane Separation. *Springer Series on Polymer and Composite Materials*, **2021**, 113-144	0.9	3
56	Hexagonal Boron Nitride (h-BN) in Solutes Separation. *Springer Series on Polymer and Composite Materials*, **2021**, 163-191	0.9	2
55	The removal of nitrogen monoxide from polluted air using CHA- and DDR-type zeolite membranes: Insights from molecular simulations. *Materials Today Communications*, **2021**, 28, 102651	2.5	2
54	From excess to absolute adsorption isotherm: The effect of the adsorbed density. *Chemical Engineering Journal*, **2021**, 425, 131495	14.7	4
53	Investigation of OH radical in the water nanodroplet during vapor freezing process: An ab initio molecular dynamics study. *Journal of Molecular Liquids*, **2021**, 343, 117597	6	1
52	Functionalized boron nitride nanosheet as a membrane for removal of Pb2+ and Cd2+ ions from aqueous solution. *Journal of Molecular Liquids*, **2021**, 321, 114920	6	5

51	Atomistic understanding of functionalized Ⅱ-graphyne-1 nanosheet membranes for water desalination. *Journal of Membrane Science*, **2020**, 604, 118079	9.6	15
50	Separation of noble gases using CHA-type zeolite membrane: insights from molecular dynamics simulation. *Chemical Papers*, **2020**, 74, 3057-3065	1.9	10
49	Computational study on the removal of trihalomethanes from water using functionalized graphene oxide membranes. *Chemical Physics*, **2020**, 531, 110589	2.3	7
48	Separation of methane from different gas mixtures using modified silicon carbide nanosheet: Micro and macro scale numerical studies. *Chinese Journal of Chemical Engineering*, **2020**, 28, 1268-1276	3.2	3
47	Molecular insights into water desalination performance of pristine graphdiyne nanosheet membrane. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107729	2.8	8
46	Water desalination across functionalized silicon carbide nanosheet membranes: insights from molecular simulations. *Structural Chemistry*, **2020**, 31, 293-303	1.8	10
45	Molecular dynamics simulation of water purification using zeolite MFI nanosheets. *Separation and Purification Technology*, **2020**, 234, 116080	8.3	21
44	Molecular dynamics study for CH4/H2S separation through functionalized nanoporous graphyne membrane. *Petroleum Science and Technology*, **2019**, 37, 2043-2048	1.4	2
43	Selective separation of methanol-water mixture using functionalized boron nitride nanosheet membrane: a computer simulation study. *Structural Chemistry*, **2019**, 30, 1451-1457	1.8	5
42	Molecular insights into effective water desalination through functionalized nanoporous boron nitride nanosheet membranes. *Applied Surface Science*, **2019**, 471, 921-928	6.7	29
41	Separation of perchlorates from aqueous solution using functionalized graphene oxide nanosheets: a computational study. *Journal of Materials Science*, **2019**, 54, 2289-2299	4.3	13
40	Water desalination through fluorine-functionalized nanoporous graphene oxide membranes. *Materials Chemistry and Physics*, **2019**, 223, 277-286	4.4	20
39	Improving the performance of water desalination through ultra-permeable functionalized nanoporous graphene oxide membrane. *Applied Surface Science*, **2018**, 427, 1000-1008	6.7	44
38	Fluorine-functionalized nanoporous graphene as an effective membrane for water desalination. *Structural Chemistry*, **2018**, 29, 1845-1852	1.8	17
37	Computational study on the efficiency of MoS 2 membrane for removing arsenic from contaminated water. *Journal of Molecular Liquids*, **2018**, 249, 110-116	6	32
36	Separation of CH4/C2H6 Mixture Using Functionalized Nanoporous Silicon Carbide Nanosheet. *Energy & Fuels*, **2018**, 32, 7508-7518	4.1	6
35	Computational study on the ability of functionalized graphene nanosheet for nitrate removal from water. *Chemical Physics*, **2018**, 511, 20-26	2.3	15
34	MoS2 nanosheet as a promising nanostructure membrane for gas separation. *Journal of Industrial and Engineering Chemistry*, **2018**, 66, 269-278	6.3	15

33	Separation of cyanide from an aqueous solution using armchair silicon carbide nanotubes: insights from molecular dynamics simulations. *RSC Advances*, **2017**, 7, 7502-7508	3.7	2
32	Molecular dynamics simulation of salt rejection through silicon carbide nanotubes as a nanostructure membrane. *Journal of Molecular Graphics and Modelling*, **2017**, 71, 176-183	2.8	22
31	Improving the performance of heavy metal separation from water using MoS2 membrane: Molecular dynamics simulation. *Computational Materials Science*, **2017**, 137, 201-207	3.2	25
30	Molecular dynamics simulations of removal of cyanide from aqueous solution using boron nitride nanotubes. *Computational Materials Science*, **2017**, 128, 8-14	3.2	11
29	Molecular Dynamics Simulation Study of the HIV-1 Protease Inhibit ion Using Fullerene and New Fullerene Derivatives of Carbon Nanostructures. *Mini-Reviews in Medicinal Chemistry*, **2017**, 17, 633-647	3.2	10
28	Removal of nitrate ion from water using boron nitride nanotubes: Insights from molecular dynamics simulations. *Computational and Theoretical Chemistry*, **2016**, 1098, 56-62	2	13
27	Molecular dynamics simulation of transport of water/DMSO and water/acetone mixtures through boron nitride nanotube. *Fluid Phase Equilibria*, **2016**, 425, 230-236	2.5	15
26	A theoretical study of nanostructure membranes for separating Li+ and Mg2+ from Cl *Computational Materials Science*, **2016**, 113, 66-74	3.2	8
25	Molecular dynamics simulation of non-covalent single-walled carbon nanotube functionalization with surfactant peptides. *Journal of Molecular Graphics and Modelling*, **2016**, 64, 75-84	2.8	26
24	Molecular dynamics simulations of trihalomethanes removal from water using boron nitride nanosheets. *Journal of Molecular Modeling*, **2016**, 22, 82	2	22
23	Separation of copper and mercury as heavy metals from aqueous solution using functionalized boron nitride nanosheets: A theoretical study. *Journal of Molecular Structure*, **2016**, 1108, 144-149	3.4	25
22	Ab Initio Study of Structure Pyridinium-Based Ionic Liquids and Derivatives. *Quantum Matter*, **2016**, 5, 53-57		2
21	Separation of nitrate ion from water using silicon carbide nanotubes as a membrane: Insights from molecular dynamics simulation. *Computational Materials Science*, **2016**, 119, 74-81	3.2	18
20	Functionalized Graphene Nanosheet as a Membrane for Water Desalination Using Applied Electric Fields: Insights from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 23883-23891	3.8	59
19	Separation of carbon dioxide and nitrogen gases through modified boron nitride nanosheets as a membrane: insights from molecular dynamics simulations. *RSC Advances*, **2016**, 6, 94911-94920	3.7	30
18	Removal of a hazardous heavy metal from aqueous solution using functionalized graphene and boron nitride nanosheets: Insights from simulations. *Journal of Molecular Graphics and Modelling*, **2015**, 61, 13-20	2.8	43
17	Removal of heavy metals from water through armchair carbon and boron nitride nanotubes: a computer simulation study. *RSC Advances*, **2015**, 5, 25097-25104	3.7	23
16	Molecular dynamics simulation of ion separation and water transport through boron nitride nanotubes. *Desalination and Water Treatment*, **2015**, 56, 1090-1098		5

15	Molecular Dynamics Simulation of Nanoporous Graphene as Membrane for Ion Separation Under Induced Electric Field. *Journal of Computational and Theoretical Nanoscience*, **2015**, 12, 1512-1518	0.3	4
14	Molecular dynamics simulation of trihalomethanes separation from water by functionalized nanoporous graphene under induced pressure. *Chemical Engineering Science*, **2015**, 127, 285-292	4.4	58
13	Removal of trihalomethanes from aqueous solution through armchair carbon nanotubes: a molecular dynamics study. *Journal of Molecular Graphics and Modelling*, **2015**, 57, 70-5	2.8	14
12	The permeation of potassium and chloride ions through nanotubes: a molecular simulation study. *Monatshefte F□ Chemie*, **2014**, 145, 881-890	1.4	16
11	Water desalination through armchair carbon nanotubes: a molecular dynamics study. *RSC Advances*, **2014**, 4, 63712-63718	3.7	27
10	Separation of a heavy metal from water through a membrane containing boron nitride nanotubes: molecular dynamics simulations. *Journal of Molecular Modeling*, **2014**, 20, 2468	2	23
9	Functionalized graphene as a nanostructured membrane for removal of copper and mercury from aqueous solution: a molecular dynamics simulation study. *Journal of Molecular Graphics and Modelling*, **2014**, 53, 112-117	2.8	44
8	Ion and Water Transport Through (7, 7) and (8, 8) Carbon and Boron Nitride Nanotubes of Different Electric Fields: A Molecular Dynamics Simulation Study. *Journal of Computational and Theoretical Nanoscience*, **2014**, 11, 2611-2617	0.3	8
7	Isopiestic studies of thermodynamic properties of solutions of ampicillin sodium and penicillin sodium in water at T = 298.15 K. *Fluid Phase Equilibria*, **2013**, 338, 204-208	2.5	1
6	COMPARATIVE INVESTIGATION OF THE EFFECT OF TYPE OF DENSITY FUNCTIONAL IN THE DETERMINATION OF GEOMETRICAL PARAMETERS IN A Cu COMPLEX. *Journal of Theoretical and Computational Chemistry*, **2013**, 12, 1350066	1.8	2
5	Isopiestic determination of the osmotic coefficient and vapour pressure of N-R-4-(N,N-dimethylamino)pyridinium tetrafluoroborate (R = C4H9, C5H11, C6H13) in the ethanol solution at T = 298.15 K. *Journal of Chemical Thermodynamics*, **2012**, 49, 70-74	2.9	3
4	The preferential permeation of ions across carbon and boron nitride nanotubes. *Chemical Physics*, **2012**, 403, 105-112	2.3	21
3	Isopiestic study of mixed electrolyte solution {yCuCl2+(1□)CaCl2} in ethanol at T=298.15K. *Fluid Phase Equilibria*, **2012**, 322-323, 1-8	2.5	1
2	Osmotic and activity coefficients in the binary solutions of 1-butyl-3-methylimidazolium chloride and bromide in methanol or ethanol at T = 298.15 K from isopiestic measurements. *Journal of Chemical Thermodynamics*, **2011**, 43, 1886-1892	2.9	9
1	Theoretical Study of CO2/N2 Gas Mixture Separation through a High-Silica PWN-type Zeolite Membrane. *Industrial & Engineering Chemistry Research*,	3.9	2