

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Functionalized Graphene Nanosheet as a Membrane for Water Desalination Using Applied Electric Fields: Insights from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 23883-23891	3.8	59
67	Molecular dynamics simulation of trihalomethanes separation from water by functionalized nanoporous graphene under induced pressure. <i>Chemical Engineering Science</i> , <b>2015</b> , 127, 285-292	4.4	58
66	Improving the performance of water desalination through ultra-permeable functionalized nanoporous graphene oxide membrane. <i>Applied Surface Science</i> , <b>2018</b> , 427, 1000-1008	6.7	44
65	Functionalized graphene as a nanostructured membrane for removal of copper and mercury from aqueous solution: a molecular dynamics simulation study. <i>Journal of Molecular Graphics and Modelling</i> , <b>2014</b> , 53, 112-117	2.8	44
64	Removal of a hazardous heavy metal from aqueous solution using functionalized graphene and boron nitride nanosheets: Insights from simulations. <i>Journal of Molecular Graphics and Modelling</i> , <b>2015</b> , 61, 13-20	2.8	43
63	Computational study on the efficiency of MoS <sub>2</sub> membrane for removing arsenic from contaminated water. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 249, 110-116	6	32
62	Separation of carbon dioxide and nitrogen gases through modified boron nitride nanosheets as a membrane: insights from molecular dynamics simulations. <i>RSC Advances</i> , <b>2016</b> , 6, 94911-94920	3.7	30
61	Molecular insights into effective water desalination through functionalized nanoporous boron nitride nanosheet membranes. <i>Applied Surface Science</i> , <b>2019</b> , 471, 921-928	6.7	29
60	Water desalination through armchair carbon nanotubes: a molecular dynamics study. <i>RSC Advances</i> , <b>2014</b> , 4, 63712-63718	3.7	27
59	Molecular dynamics simulation of non-covalent single-walled carbon nanotube functionalization with surfactant peptides. <i>Journal of Molecular Graphics and Modelling</i> , <b>2016</b> , 64, 75-84	2.8	26
58	Separation of copper and mercury as heavy metals from aqueous solution using functionalized boron nitride nanosheets: A theoretical study. <i>Journal of Molecular Structure</i> , <b>2016</b> , 1108, 144-149	3.4	25
57	Improving the performance of heavy metal separation from water using MoS <sub>2</sub> membrane: Molecular dynamics simulation. <i>Computational Materials Science</i> , <b>2017</b> , 137, 201-207	3.2	25
56	Removal of heavy metals from water through armchair carbon and boron nitride nanotubes: a computer simulation study. <i>RSC Advances</i> , <b>2015</b> , 5, 25097-25104	3.7	23
55	Separation of a heavy metal from water through a membrane containing boron nitride nanotubes: molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2468	2	23
54	Molecular dynamics simulation of salt rejection through silicon carbide nanotubes as a nanostructure membrane. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 71, 176-183	2.8	22
53	Molecular dynamics simulations of trihalomethanes removal from water using boron nitride nanosheets. <i>Journal of Molecular Modeling</i> , <b>2016</b> , 22, 82	2	22
52	The preferential permeation of ions across carbon and boron nitride nanotubes. <i>Chemical Physics</i> , <b>2012</b> , 403, 105-112	2.3	21

51	Molecular dynamics simulation of water purification using zeolite MFI nanosheets. <i>Separation and Purification Technology</i> , <b>2020</b> , 234, 116080	8.3	21
50	Water desalination through fluorine-functionalized nanoporous graphene oxide membranes. <i>Materials Chemistry and Physics</i> , <b>2019</b> , 223, 277-286	4.4	20
49	Separation of nitrate ion from water using silicon carbide nanotubes as a membrane: Insights from molecular dynamics simulation. <i>Computational Materials Science</i> , <b>2016</b> , 119, 74-81	3.2	18
48	Fluorine-functionalized nanoporous graphene as an effective membrane for water desalination. <i>Structural Chemistry</i> , <b>2018</b> , 29, 1845-1852	1.8	17
47	The permeation of potassium and chloride ions through nanotubes: a molecular simulation study. <i>Monatshefte für Chemie</i> , <b>2014</b> , 145, 881-890	1.4	16
46	Atomistic understanding of functionalized Graphyne-1 nanosheet membranes for water desalination. <i>Journal of Membrane Science</i> , <b>2020</b> , 604, 118079	9.6	15
45	Molecular dynamics simulation of transport of water/DMSO and water/acetone mixtures through boron nitride nanotube. <i>Fluid Phase Equilibria</i> , <b>2016</b> , 425, 230-236	2.5	15
44	Computational study on the ability of functionalized graphene nanosheet for nitrate removal from water. <i>Chemical Physics</i> , <b>2018</b> , 511, 20-26	2.3	15
43	MoS <sub>2</sub> nanosheet as a promising nanostructure membrane for gas separation. <i>Journal of Industrial and Engineering Chemistry</i> , <b>2018</b> , 66, 269-278	6.3	15
42	Removal of trihalomethanes from aqueous solution through armchair carbon nanotubes: a molecular dynamics study. <i>Journal of Molecular Graphics and Modelling</i> , <b>2015</b> , 57, 70-5	2.8	14
41	Removal of nitrate ion from water using boron nitride nanotubes: Insights from molecular dynamics simulations. <i>Computational and Theoretical Chemistry</i> , <b>2016</b> , 1098, 56-62	2	13
40	Separation of perchlorates from aqueous solution using functionalized graphene oxide nanosheets: a computational study. <i>Journal of Materials Science</i> , <b>2019</b> , 54, 2289-2299	4.3	13
39	Molecular dynamics simulations of removal of cyanide from aqueous solution using boron nitride nanotubes. <i>Computational Materials Science</i> , <b>2017</b> , 128, 8-14	3.2	11
38	Separation of noble gases using CHA-type zeolite membrane: insights from molecular dynamics simulation. <i>Chemical Papers</i> , <b>2020</b> , 74, 3057-3065	1.9	10
37	Molecular Dynamics Simulation Study of the HIV-1 Protease Inhibit ion Using Fullerene and New Fullerene Derivatives of Carbon Nanostructures. <i>Mini-Reviews in Medicinal Chemistry</i> , <b>2017</b> , 17, 633-647	3.2	10
36	Water desalination across functionalized silicon carbide nanosheet membranes: insights from molecular simulations. <i>Structural Chemistry</i> , <b>2020</b> , 31, 293-303	1.8	10
35	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. <i>Journal of Chemical Thermodynamics</i> , <b>2011</b> , 43, 1886-1892	2.9	9
34	A theoretical study of nanostructure membranes for separating Li <sup>+</sup> and Mg <sup>2+</sup> from Cl <sup>-</sup> . <i>Computational Materials Science</i> , <b>2016</b> , 113, 66-74	3.2	8

33	Ion and Water Transport Through (7, 7) and (8, 8) Carbon and Boron Nitride Nanotubes of Different Electric Fields: A Molecular Dynamics Simulation Study. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2014</b> , 11, 2611-2617	0.3	8
32	Molecular insights into water desalination performance of pristine graphdiyne nanosheet membrane. <i>Journal of Molecular Graphics and Modelling</i> , <b>2020</b> , 101, 107729	2.8	8
31	Computational study on the removal of trihalomethanes from water using functionalized graphene oxide membranes. <i>Chemical Physics</i> , <b>2020</b> , 531, 110589	2.3	7
30	Separation of CH <sub>4</sub> /C <sub>2</sub> H <sub>6</sub> Mixture Using Functionalized Nanoporous Silicon Carbide Nanosheet. <i>Energy &amp; Fuels</i> , <b>2018</b> , 32, 7508-7518	4.1	6
29	Selective separation of methanol-water mixture using functionalized boron nitride nanosheet membrane: a computer simulation study. <i>Structural Chemistry</i> , <b>2019</b> , 30, 1451-1457	1.8	5
28	Molecular dynamics simulation of ion separation and water transport through boron nitride nanotubes. <i>Desalination and Water Treatment</i> , <b>2015</b> , 56, 1090-1098		5
27	Atomistic understanding of gas separation through nanoporous DDR-type zeolite membrane. <i>Chemical Physics</i> , <b>2021</b> , 540, 110985	2.3	5
26	Theoretical investigation of the removal of nitrate ions from contaminated aqueous solution using functionalized silicon carbide nanosheets. <i>Computational Materials Science</i> , <b>2021</b> , 187, 110118	3.2	5
25	Functionalized boron nitride nanosheet as a membrane for removal of Pb <sup>2+</sup> and Cd <sup>2+</sup> ions from aqueous solution. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 321, 114920	6	5
24	Molecular Dynamics Simulation of Nanoporous Graphene as Membrane for Ion Separation Under Induced Electric Field. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2015</b> , 12, 1512-1518	0.3	4
23	Molecular dynamics simulation of separation of water/methanol and water/ethanol mixture using boron nitride nanotubes. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 331, 115774	6	4
22	From excess to absolute adsorption isotherm: The effect of the adsorbed density. <i>Chemical Engineering Journal</i> , <b>2021</b> , 425, 131495	14.7	4
21	Isopestic determination of the osmotic coefficient and vapour pressure of N-R-4-(N,N-dimethylamino)pyridinium tetrafluoroborate (R = C <sub>4</sub> H <sub>9</sub> , C <sub>5</sub> H <sub>11</sub> , C <sub>6</sub> H <sub>13</sub> ) in the ethanol solution at T = 298.15 K. <i>Journal of Chemical Thermodynamics</i> , <b>2012</b> , 49, 70-74	2.9	3
20	Efficient water desalination through mono and bilayer carbon nitride nanosheet membranes: Insights from molecular dynamics simulation. <i>Journal of Molecular Graphics and Modelling</i> , <b>2022</b> , 110, 108059	2.8	3
19	Separation of methane from different gas mixtures using modified silicon carbide nanosheet: Micro and macro scale numerical studies. <i>Chinese Journal of Chemical Engineering</i> , <b>2020</b> , 28, 1268-1276	3.2	3
18	Graphene Oxide and Reduced Graphene Oxide as Nanofillers in Membrane Separation. <i>Springer Series on Polymer and Composite Materials</i> , <b>2021</b> , 113-144	0.9	3
17	Separation of cyanide from an aqueous solution using armchair silicon carbide nanotubes: insights from molecular dynamics simulations. <i>RSC Advances</i> , <b>2017</b> , 7, 7502-7508	3.7	2
16	Molecular dynamics study for CH <sub>4</sub> /H <sub>2</sub> S separation through functionalized nanoporous graphyne membrane. <i>Petroleum Science and Technology</i> , <b>2019</b> , 37, 2043-2048	1.4	2

15	COMPARATIVE INVESTIGATION OF THE EFFECT OF TYPE OF DENSITY FUNCTIONAL IN THE DETERMINATION OF GEOMETRICAL PARAMETERS IN A Cu COMPLEX. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2013</b> , 12, 1350066	1.8	2
14	Separation of CH <sub>4</sub> /N <sub>2</sub> gas mixture using MFI zeolite nanosheet: Insights from molecular dynamics simulation. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , <b>2022</b> , 641, 128527	5.1	2
13	Ab Initio Study of Structure Pyridinium-Based Ionic Liquids and Derivatives. <i>Quantum Matter</i> , <b>2016</b> , 5, 53-57		2
12	Molecular insight into water desalination through functionalized graphenylene nanosheet membranes. <i>Computational Materials Science</i> , <b>2022</b> , 203, 111126	3.2	2
11	Hexagonal Boron Nitride (h-BN) in Solutes Separation. <i>Springer Series on Polymer and Composite Materials</i> , <b>2021</b> , 163-191	0.9	2
10	The removal of nitrogen monoxide from polluted air using CHA- and DDR-type zeolite membranes: Insights from molecular simulations. <i>Materials Today Communications</i> , <b>2021</b> , 28, 102651	2.5	2
9	Theoretical Study of CO <sub>2</sub> /N <sub>2</sub> Gas Mixture Separation through a High-Silica PWN-type Zeolite Membrane. <i>Industrial &amp; Engineering Chemistry Research</i> ,	3.9	2
8	Isopiestic studies of thermodynamic properties of solutions of ampicillin sodium and penicillin sodium in water at T = 298.15 K. <i>Fluid Phase Equilibria</i> , <b>2013</b> , 338, 204-208	2.5	1
7	Isopiestic study of mixed electrolyte solution {yCuCl <sub>2</sub> +(1-y)CaCl <sub>2</sub> } in ethanol at T=298.15K. <i>Fluid Phase Equilibria</i> , <b>2012</b> , 322-323, 1-8	2.5	1
6	Efficient Removal of Heavy Metals from Aqueous Solutions through Functionalized EGraphyne-1 Membranes under External Uniform Electric Fields: Insights from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 12254-12263	3.4	1
5	Investigation of OH radical in the water nanodroplet during vapor freezing process: An ab initio molecular dynamics study. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 343, 117597	6	1
4	A theoretical investigation into the effects of functionalized graphene nanosheets on dimethyl sulfoxide separation.. <i>Chemosphere</i> , <b>2022</b> , 134183	8.4	1
3	The performance of a C <sub>2</sub> N membrane for heavy metal ions removal from water under external electric field. <i>Separation and Purification Technology</i> , <b>2022</b> , 289, 120770	8.3	0
2	A new insight into the interaction of hydroxyl radical with supercooled nanodroplet in the atmosphere. <i>Journal of Molecular Liquids</i> , <b>2022</b> , 359, 119261	6	0
1	Efficient separation of He/CH <sub>4</sub> mixture by functionalized graphenylene membranes: A theoretical study.. <i>Journal of Molecular Graphics and Modelling</i> , <b>2022</b> , 115, 108211	2.8	0