

Sohail Murad

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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.

80
papers

1,717
citations

23
h-index

38
g-index

82
ext. papers

1,891
ext. citations

3.3
avg, IF

4.9
L-index

#	Paper	IF	Citations
80	Singularity free algorithm for molecular dynamics simulation of rigid polyatomics. <i>Molecular Physics</i> , 1977 , 34, 327-331	1.7	398
79	A molecular dynamics simulation of droplet evaporation. <i>International Journal of Heat and Mass Transfer</i> , 2003 , 46, 3179-3188	4.9	76
78	Influence of hydrophilic surface specificity on the structural properties of confined water. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 13825-39	3.4	69
77	Thermal transport across nanoscale solid-fluid interfaces. <i>Applied Physics Letters</i> , 2008 , 92, 133105	3.4	66
76	Aromatic Polyamide Reverse-Osmosis Membrane: An Atomistic Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 10311-10318	3.4	59
75	Molecular simulation of thermal transport across hydrophilic interfaces. <i>Chemical Physics Letters</i> , 2008 , 467, 110-113	2.5	48
74	Thermal conductivity in molecular fluids. <i>Molecular Physics</i> , 1989 , 68, 1219-1223	1.7	42
73	Zeolite-fiber integrated optical chemical sensors for detection of dissolved organics in water. <i>Langmuir</i> , 2005 , 21, 8609-12	4	41
72	Preferential ion and water intake using charged carbon nanotubes. <i>Chemical Physics Letters</i> , 2007 , 434, 292-296	2.5	40
71	Nanoparticle permeation induces water penetration, ion transport, and lipid flip-flop. <i>Langmuir</i> , 2012 , 28, 16989-7000	4	34
70	Molecular dynamics simulation of ion selectivity process in nanopores. <i>Molecular Simulation</i> , 2008 , 34, 169-175	2	34
69	The role of external electric fields in enhancing ion mobility, drift velocity, and drift-diffusion rates in aqueous electrolyte solutions. <i>Journal of Chemical Physics</i> , 2011 , 134, 114504	3.9	33
68	Permeation of nanocrystals across lipid membranes. <i>Molecular Physics</i> , 2011 , 109, 1511-1526	1.7	30
67	Surface-functionalized nanoparticle permeation triggers lipid displacement and water and ion leakage. <i>Langmuir</i> , 2015 , 31, 1074-85	4	28
66	Thermal transport through a fluid-solid interface. <i>Chemical Physics Letters</i> , 2009 , 476, 267-270	2.5	28
65	Role of surface ligands in nanoparticle permeation through a model membrane: a coarse-grained molecular dynamics simulations study. <i>Molecular Physics</i> , 2012 , 110, 2181-2195	1.7	28
64	Molecular dynamics averaging of Xe chemical shifts in liquids. <i>Journal of Chemical Physics</i> , 2004 , 121, 9581-92	3.9	28

63	Xenon Recovery by DD3R Zeolite Membranes: Application in Anaesthetics. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 15518-15525	16.4	27
62	Understanding the effect of zeolite crystal expansion/contraction on separation performance of NaA zeolite membrane: A combined experimental and molecular simulation study. <i>Journal of Membrane Science</i> , 2017 , 539, 14-23	9.6	25
61	A simple molecular dynamics simulation for calculating Henry's constant and solubility of gases in liquids. <i>Chemical Physics Letters</i> , 2000 , 319, 60-64	2.5	25
60	The structure of hydrogen chloride. <i>Molecular Physics</i> , 1984 , 51, 525-529	1.7	24
59	Proton-Selective Ion Transport in ZSM-5 Zeolite Membrane. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 26386-26392	3.8	23
58	The Composition of the Mobile Phase Affects the Dynamic Chiral Recognition of Drug Molecules by the Chiral Stationary Phase. <i>Langmuir</i> , 2017 , 33, 11246-11256	4	23
57	Transport of Vanadium and Oxovanadium Ions Across Zeolite Membranes: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 23803-23810	3.8	22
56	The effect of thickness, pore size and structure of a nanomembrane on the flux and selectivity in reverse osmosis separations: a molecular dynamics study. <i>Chemical Physics Letters</i> , 2004 , 397, 211-215	2.5	22
55	Zeolite membranes for ion separations from aqueous solutions. <i>Current Opinion in Chemical Engineering</i> , 2015 , 8, 15-20	5.4	21
54	A thermal logic device based on fluid-solid interfaces. <i>Applied Physics Letters</i> , 2013 , 102, 193109	3.4	21
53	Communication: Thermal rectification in liquids by manipulating the solid-liquid interface. <i>Journal of Chemical Physics</i> , 2012 , 137, 081101	3.9	21
52	Simulated Permeation and Characterization of PEGylated Gold Nanoparticles in a Lipid Bilayer System. <i>Langmuir</i> , 2016 , 32, 7541-55	4	19
51	Nanoscale jet collision and mixing dynamics. <i>Nano Letters</i> , 2007 , 7, 707-12	11.5	18
50	Molecular dynamics simulations of the chiral recognition mechanism for a polysaccharide chiral stationary phase in enantiomeric chromatographic separations. <i>Molecular Physics</i> , 2019 , 117, 3569-3588	1.7	17
49	Dynamics of nanoscale jet formation and impingement on flat surfaces. <i>Physics of Fluids</i> , 2007 , 19, 128102	4.4	17
48	Hydration of ions under confinement. <i>Molecular Simulation</i> , 2010 , 36, 579-589	2	16
47	Thermal rectification in a fluid reservoir. <i>Applied Physics Letters</i> , 2012 , 100, 121901	3.4	16
46	Structure of aqueous MgSO ₄ solution: Dilute to concentrated. <i>Chemical Physics Letters</i> , 2011 , 508, 38-42	2.5	14

45	Thermal transport through superlattice solid-solid interfaces. <i>Applied Physics Letters</i> , 2009 , 95, 051907	3.4	14
44	Fabrication and stability exploration of hollow fiber mordenite zeolite membranes for isopropanol/water mixture separation. <i>Microporous and Mesoporous Materials</i> , 2019 , 274, 347-355	5.3	14
43	Crystallization of acetaminophen on chitosan films blended with different acids. <i>Chemical Engineering Science</i> , 2015 , 126, 1-9	4.4	13
42	Exploring gas permeability of lipid membranes using coarse-grained molecular dynamics. <i>Molecular Simulation</i> , 2009 , 35, 953-961	2	13
41	Rotational behaviour of PEGylated gold nanorods in a lipid bilayer system. <i>Molecular Physics</i> , 2017 , 115, 1122-1143	1.7	12
40	Diffusion of gases across lipid membranes with OmpA channel: a molecular dynamics study. <i>Molecular Physics</i> , 2010 , 108, 1569-1581	1.7	12
39	Molecular Dynamics Simulations of Xe Chemical Shifts and Solubility in Alkanes. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 15771-15783	3.8	12
38	Modeling Enantiomeric Separations as an Interfacial Process Using Amylose Tris(3,5-dimethylphenyl carbamate) (ADMPC) Polymers Coated on Amorphous Silica. <i>Langmuir</i> , 2020 , 36, 1113-1124	4	12
37	Molecular dynamics simulations of liquid-liquid phase equilibrium of ternary methanol/water/hydrocarbon mixtures. <i>Fluid Phase Equilibria</i> , 2018 , 470, 109-119	2.5	12
36	Computational Molecular Modeling of Transport Processes in Nanoporous Membranes. <i>Processes</i> , 2018 , 6, 124	2.9	12
35	Dynamic rectification in a thermal diode based on fluid-solid interfaces: Contrasting behavior of soft materials and fluids. <i>Applied Physics Letters</i> , 2014 , 104, 211601	3.4	11
34	Molecular dynamics simulations reveal how characteristics of surface and permeant affect permeation events at the surface of soft matter. <i>Molecular Simulation</i> , 2017 , 43, 439-466	2	9
33	Atomistic Simulations of Biofouling and Molecular Transfer of a Cross-linked Aromatic Polyamide Membrane for Desalination. <i>Langmuir</i> , 2020 , 36, 7658-7668	4	8
32	Xenon Recovery by DD3R Zeolite Membranes: Application in Anaesthetics. <i>Angewandte Chemie</i> , 2019 , 131, 15664-15671	3.6	8
31	Communication: A tractable design for a thermal transistor. <i>Journal of Chemical Physics</i> , 2013 , 139, 151102	1.9	8
30	Prediction of Henry's constants of xenon in cyclo-alkanes from molecular dynamics simulations. <i>Fluid Phase Equilibria</i> , 2008 , 269, 73-79	2.5	8
29	Prediction of hydrogen solubility in heavy hydrocarbons over a range of temperatures and pressures using molecular dynamics simulations. <i>Fluid Phase Equilibria</i> , 2010 , 299, 94-101	2.5	7
28	Simulations of the Thermal Conductivity in the Vicinity of the Critical Point. <i>Molecular Simulation</i> , 1998 , 20, 385-395	2	7

27	Molecular simulations of the competitive adsorption of siloxanes and water on amorphous silica surfaces as a function of temperature. <i>Chemical Physics Letters</i> , 2011 , 516, 216-219	2.5	6
26	Anomalous flow behavior in nanochannels: A molecular dynamics study. <i>Chemical Physics Letters</i> , 2010 , 492, 285-289	2.5	6
25	Understanding unusual thermal transport behavior in soft materials under mechanical strain [A molecular dynamics study. <i>Chemical Physics Letters</i> , 2015 , 626, 102-105	2.5	5
24	Using Molecular Simulations To Develop Reliable Design Tools and Correlations for Engineering Applications of Aqueous Electrolyte Solutions. <i>Journal of Chemical & Engineering Data</i> , 2016 , 61, 1578-1584	2.8	5
23	Evaluation and extrapolation of the solubility of H ₂ and CO in n-alkanes and n-alcohols using molecular simulation. <i>Fluid Phase Equilibria</i> , 2014 , 384, 43-49	2.5	5
22	Effect of Phosphate Salt Concentration and Solution pH on the Aqueous-Phase Homo and Copolymerization of N-Vinyl Pyrrolidone. <i>Macromolecular Reaction Engineering</i> , 2018 , 12, 1800012	1.5	5
21	Molecular Dynamics Studies of Nanoparticle Transport Through Model Lipid Membranes 2019 , 109-165		4
20	Achieving thermal rectification in designed liquid-liquid systems. <i>Applied Physics Letters</i> , 2016 , 108, 134104		4
19	Molecular simulations of thermal transport across interfaces: solid-liquid and solid-solid. <i>Molecular Simulation</i> , 2012 , 38, 642-652	2	4
18	Anomalous flow behavior in closed and open thin walled nanochannels. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010 , 374, 4242-4246	2.3	4
17	Heat induced polarization in molecular fluids. <i>Molecular Physics</i> , 1990 , 69, 697-702	1.7	4
16	How the capillarity and ink-air flow govern the performance of a fountain pen. <i>Journal of Colloid and Interface Science</i> , 2020 , 578, 660-667	9.3	3
15	A GENERALIZED CORRESPONDING STATES THEORY FOR THE SURFACE TENSION OF LIQUIDS AND LIQUID MIXTURES. <i>Chemical Engineering Communications</i> , 1986 , 40, 345-358	2.2	3
14	Molecular-Level "Observations" of the Behavior of Gold Nanoparticles in Aqueous Solution and Interacting with a Lipid Bilayer Membrane. <i>Methods in Molecular Biology</i> , 2019 , 2000, 303-359	1.4	2
13	Interfacial Thermal Conductivity and Its Anisotropy. <i>Processes</i> , 2020 , 8, 27	2.9	1
12	Understanding the liquid-liquid (water-hexane) interface. <i>Chemical Physics Letters</i> , 2017 , 685, 422-426	2.5	1
11	Note: the role of external electric fields in enhancing ion mobility, drift velocity, and drift-diffusion rates in aqueous electrolyte solutions [J. Chem. Phys. 134, 114504 (2011)]. <i>Journal of Chemical Physics</i> , 2012 , 136, 076101	3.9	1
10	Capillary Flow of Power-Law Non-Newtonian Liquids in Circular Tubes. <i>Chemical Engineering Communications</i> , 2005 , 192, 575-580	2.2	1

9	Prediction of thermal conductivity for dense fluids and fluid mixtures. <i>AIChE Journal</i> , 1981 , 27, 864-866	3.6	1
8	Second-order perturbation theory for the angular correlation function of non-linear molecules. <i>Chemical Physics Letters</i> , 1981 , 84, 114-118	2.5	1
7	On using the anisotropy in the thermal resistance of solid-liquid interfaces to more effectively cool nano-electronics. <i>Molecular Simulation</i> , 2020 , 46, 162-167	2	1
6	Molecular dynamics simulations of chiral recognition of drugs by amylose polymers coated on amorphous silica. <i>Molecular Physics</i> , e1922772	1.7	1
5	Altering thermal transport by strained-layer epitaxy. <i>Applied Physics Letters</i> , 2018 , 112, 194101	3.4	1
4	Molecular dynamics simulations of enantiomeric separations as an interfacial process in HPLC. <i>AIChE Journal</i> , 2021 , 67, e17143	3.6	1
3	Novel methods to characterise spatial distribution and enantiomeric composition of usnic acids in four Icelandic lichens.. <i>Phytochemistry</i> , 2022 , 113210	4	1
2	Research Possibilities in Computational Modeling as a Low Cost Alternative to Traditional Experimental Research 2022 , 165-172		
1	Understanding Separation Mechanisms of Monoatomic Gases, Such as Kr and Xe, via DD3R Zeolite Membrane Using Molecular Dynamics. <i>Thermo</i> , 2022 , 2, 56-73		