Sohail Murad

List of Publications by Year in Descending Order

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	Research Possibilities in Computational Modeling as a Low Cost Alternative to Traditional Experimental Research **2022**, 165-172		
79	Understanding Separation Mechanisms of Monoatomic Gases, Such as Kr and Xe, via DD3R Zeolite Membrane Using Molecular Dynamics. *Thermo*, **2022**, 2, 56-73		
78	Novel methods to characterise spatial distribution and enantiomeric composition of usnic acids in four Icelandic lichens.. *Phytochemistry*, **2022**, 113210	4	1
77	Molecular dynamics simulations of enantiomeric separations as an interfacial process in HPLC. *AICHE Journal*, **2021**, 67, e17143	3.6	1
76	Atomistic Simulations of Biofouling and Molecular Transfer of a Cross-linked Aromatic Polyamide Membrane for Desalination. *Langmuir*, **2020**, 36, 7658-7668	4	8
75	How the capillarity and ink-air flow govern the performance of a fountain pen. *Journal of Colloid and Interface Science*, **2020**, 578, 660-667	9.3	3
74	Interfacial Thermal Conductivity and Its Anisotropy. *Processes*, **2020**, 8, 27	2.9	1
73	Modeling Enantiomeric Separations as an Interfacial Process Using Amylose Tris(3,5-dimethylphenyl carbamate) (ADMPC) Polymers Coated on Amorphous Silica. *Langmuir*, **2020**, 36, 1113-1124	4	12
72	On using the anisotropy in the thermal resistance of solid–fluid interfaces to more effectively cool nano-electronics. *Molecular Simulation*, **2020**, 46, 162-167	2	1
71	Xenon Recovery by DD3R Zeolite Membranes: Application in Anaesthetics. *Angewandte Chemie - International Edition*, **2019**, 58, 15518-15525	16.4	27
70	Molecular-Level "Observations" of the Behavior of Gold Nanoparticles in Aqueous Solution and Interacting with a Lipid Bilayer Membrane. *Methods in Molecular Biology*, **2019**, 2000, 303-359	1.4	2
69	Molecular Dynamics Studies of Nanoparticle Transport Through Model Lipid Membranes **2019**, 109-165		4
68	Molecular dynamics simulations of the chiral recognition mechanism for a polysaccharide chiral stationary phase in enantiomeric chromatographic separations. *Molecular Physics*, **2019**, 117, 3569-3588	1.7	17
67	Xenon Recovery by DD3R Zeolite Membranes: Application in Anaesthetics. *Angewandte Chemie*, **2019**, 131, 15664-15671	3.6	8
66	Fabrication and stability exploration of hollow fiber mordenite zeolite membranes for isopropanol/water mixture separation. *Microporous and Mesoporous Materials*, **2019**, 274, 347-355	5.3	14
65	Molecular dynamics simulations of liquid-liquid phase equilibrium of ternary methanol/water/hydrocarbon mixtures. *Fluid Phase Equilibria*, **2018**, 470, 109-119	2.5	12
64	Computational Molecular Modeling of Transport Processes in Nanoporous Membranes. *Processes*, **2018**, 6, 124	2.9	12

63	Altering thermal transport by strained-layer epitaxy. *Applied Physics Letters*, **2018**, 112, 194101	3.4	1
62	Effect of Phosphate Salt Concentration and Solution pH on the Aqueous-Phase Homo and Copolymerization of N-Vinyl Pyrrolidone. *Macromolecular Reaction Engineering*, **2018**, 12, 1800012	1.5	5
61	Molecular dynamics simulations reveal how characteristics of surface and permeant affect permeation events at the surface of soft matter. *Molecular Simulation*, **2017**, 43, 439-466	2	9
60	Understanding the effect of zeolite crystal expansion/contraction on separation performance of NaA zeolite membrane: A combined experimental and molecular simulation study. *Journal of Membrane Science*, **2017**, 539, 14-23	9.6	25
59	The Composition of the Mobile Phase Affects the Dynamic Chiral Recognition of Drug Molecules by the Chiral Stationary Phase. *Langmuir*, **2017**, 33, 11246-11256	4	23
58	Understanding the liquid□liquid (water□hexane) interface. *Chemical Physics Letters*, **2017**, 685, 422-426	2.5	1
57	Rotational behaviour of PEGylated gold nanorods in a lipid bilayer system. *Molecular Physics*, **2017**, 115, 1122-1143	1.7	12
56	Aromatic Polyamide Reverse-Osmosis Membrane: An Atomistic Molecular Dynamics Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 10311-10318	3.4	59
55	Simulated Permeation and Characterization of PEGylated Gold Nanoparticles in a Lipid Bilayer System. *Langmuir*, **2016**, 32, 7541-55	4	19
54	Proton-Selective Ion Transport in ZSM-5 Zeolite Membrane. *Journal of Physical Chemistry C*, **2016**, 120, 26386-26392	3.8	23
53	Achieving thermal rectification in designed liquid-liquid systems. *Applied Physics Letters*, **2016**, 108, 134101	3.4	4
52	Using Molecular Simulations To Develop Reliable Design Tools and Correlations for Engineering Applications of Aqueous Electrolyte Solutions. *Journal of Chemical & Engineering Data*, **2016**, 61, 1578-1584	2.8	5
51	Understanding unusual thermal transport behavior in soft materials under mechanical strain □A molecular dynamics study. *Chemical Physics Letters*, **2015**, 626, 102-105	2.5	5
50	Crystallization of acetaminophen on chitosan films blended with different acids. *Chemical Engineering Science*, **2015**, 126, 1-9	4.4	13
49	Surface-functionalized nanoparticle permeation triggers lipid displacement and water and ion leakage. *Langmuir*, **2015**, 31, 1074-85	4	28
48	Zeolite membranes for ion separations from aqueous solutions. *Current Opinion in Chemical Engineering*, **2015**, 8, 15-20	5.4	21
47	Dynamic rectification in a thermal diode based on fluid-solid interfaces: Contrasting behavior of soft materials and fluids. *Applied Physics Letters*, **2014**, 104, 211601	3.4	11
46	Evaluation and extrapolation of the solubility of H2 and CO in n-alkanes and n-alcohols using molecular simulation. *Fluid Phase Equilibria*, **2014**, 384, 43-49	2.5	5

45	Transport of Vanadium and Oxovanadium Ions Across Zeolite Membranes: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2014**, 118, 23803-23810	3.8	22
44	A thermal logic device based on fluid-solid interfaces. *Applied Physics Letters*, **2013**, 102, 193109	3.4	21
43	Communication: A tractable design for a thermal transistor. *Journal of Chemical Physics*, **2013**, 139, 151102	3.9	8
42	Nanoparticle permeation induces water penetration, ion transport, and lipid flip-flop. *Langmuir*, **2012**, 28, 16989-7000	4	34
41	Communication: Thermal rectification in liquids by manipulating the solid-liquid interface. *Journal of Chemical Physics*, **2012**, 137, 081101	3.9	21
40	Role of surface ligands in nanoparticle permeation through a model membrane: a coarse-grained molecular dynamics simulations study. *Molecular Physics*, **2012**, 110, 2181-2195	1.7	28
39	Thermal rectification in a fluid reservoir. *Applied Physics Letters*, **2012**, 100, 121901	3.4	16
38	Molecular simulations of thermal transport across interfaces: solid–vapour and solid–solid. *Molecular Simulation*, **2012**, 38, 642-652	2	4
37	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)]. *Journal of Chemical Physics*, **2012**, 136, 076101	3.9	1
36	Molecular simulations of the competitive adsorption of siloxanes and water on amorphous silica surfaces as a function of temperature. *Chemical Physics Letters*, **2011**, 516, 216-219	2.5	6
35	Structure of aqueous MgSO4 solution: Dilute to concentrated. *Chemical Physics Letters*, **2011**, 508, 38-42	2.5	14
34	Permeation of nanocrystals across lipid membranes. *Molecular Physics*, **2011**, 109, 1511-1526	1.7	30
33	The role of external electric fields in enhancing ion mobility, drift velocity, and drift-diffusion rates in aqueous electrolyte solutions. *Journal of Chemical Physics*, **2011**, 134, 114504	3.9	33
32	Hydration of ions under confinement. *Molecular Simulation*, **2010**, 36, 579-589	2	16
31	Diffusion of gases across lipid membranes with OmpA channel: a molecular dynamics study. *Molecular Physics*, **2010**, 108, 1569-1581	1.7	12
30	Prediction of hydrogen solubility in heavy hydrocarbons over a range of temperatures and pressures using molecular dynamics simulations. *Fluid Phase Equilibria*, **2010**, 299, 94-101	2.5	7
29	Anomalous flow behavior in closed and open thin walled nanochannels. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2010**, 374, 4242-4246	2.3	4
28	Anomalous flow behavior in nanochannels: A molecular dynamics study. *Chemical Physics Letters*, **2010**, 492, 285-289	2.5	6

27	Thermal transport through superlattice solid-solid interfaces. *Applied Physics Letters*, **2009**, 95, 051907	3.4	14
26	Thermal transport through a fluid□solid interface. *Chemical Physics Letters*, **2009**, 476, 267-270	2.5	28
25	Influence of hydrophilic surface specificity on the structural properties of confined water. *Journal of Physical Chemistry B*, **2009**, 113, 13825-39	3.4	69
24	Exploring gas permeability of lipid membranes using coarse-grained molecular dynamics. *Molecular Simulation*, **2009**, 35, 953-961	2	13
23	Molecular dynamics simulation of ion selectivity process in nanopores. *Molecular Simulation*, **2008**, 34, 169-175	2	34
22	Thermal transport across nanoscale solid-fluid interfaces. *Applied Physics Letters*, **2008**, 92, 133105	3.4	66
21	Molecular simulation of thermal transport across hydrophilic interfaces. *Chemical Physics Letters*, **2008**, 467, 110-113	2.5	48
20	Prediction of Henry's constants of xenon in cyclo-alkanes from molecular dynamics simulations. *Fluid Phase Equilibria*, **2008**, 269, 73-79	2.5	8
19	Nanoscale jet collision and mixing dynamics. *Nano Letters*, **2007**, 7, 707-12	11.5	18
18	Molecular Dynamics Simulations of Xe Chemical Shifts and Solubility inn-Alkanes□*Journal of Physical Chemistry C*, **2007**, 111, 15771-15783	3.8	12
17	Preferential ion and water intake using charged carbon nanotubes. *Chemical Physics Letters*, **2007**, 434, 292-296	2.5	40
16	Dynamics of nanoscale jet formation and impingement on flat surfaces. *Physics of Fluids*, **2007**, 19, 128102	4	17
15	Zeolite-fiber integrated optical chemical sensors for detection of dissolved organics in water. *Langmuir*, **2005**, 21, 8609-12	4	41
14	Capillary Flow of Power-Law Non-Newtonian Liquids in Circular Tubes. *Chemical Engineering Communications*, **2005**, 192, 575-580	2.2	1
13	Molecular dynamics averaging of Xe chemical shifts in liquids. *Journal of Chemical Physics*, **2004**, 121, 9581-92	3.9	28
12	The effect of thickness, pore size and structure of a nanomembrane on the flux and selectivity in reverse osmosis separations: a molecular dynamics study. *Chemical Physics Letters*, **2004**, 397, 211-215	2.5	22
11	A molecular dynamics simulation of droplet evaporation. *International Journal of Heat and Mass Transfer*, **2003**, 46, 3179-3188	4.9	76
10	A simple molecular dynamics simulation for calculating Henry's constant and solubility of gases in liquids. *Chemical Physics Letters*, **2000**, 319, 60-64	2.5	25

9	Simulations of the Thermal Conductivity in the Vicinity of the Critical Point. *Molecular Simulation*, **1998**, 20, 385-395	2	7
8	Heat induced polarization in molecular fluids. *Molecular Physics*, **1990**, 69, 697-702	1.7	4
7	Thermal conductivity in molecular fluids. *Molecular Physics*, **1989**, 68, 1219-1223	1.7	42
6	A GENERALIZED CORRESPONDING STATES THEORY FOR THE SURFACE TENSION OF LIQUIDS AND LIQUID MIXTURES. *Chemical Engineering Communications*, **1986**, 40, 345-358	2.2	3
5	The structure of hydrogen chloride. *Molecular Physics*, **1984**, 51, 525-529	1.7	24
4	Prediction of thermal conductivity for dense fluids and fluid mixtures. *AICHE Journal*, **1981**, 27, 864-866	3.6	1
3	Second-order perturbation theory for the angular correlation function of non-linear molecules. *Chemical Physics Letters*, **1981**, 84, 114-118	2.5	1
2	Singularity free algorithm for molecular dynamics simulation of rigid polyatomics. *Molecular Physics* , **1977**, 34, 327-331	1.7	398
1	Molecular dynamics simulations of chiral recognition of drugs by amylose polymers coated on amorphous silica. *Molecular Physics*,e1922772	1.7	1