Hossein Eslami

List of Publications by Year
in descending order

51 papers	1,522 citations	236925 25 h-index	315739 38 g-index
51 all docs	51 docs citations	51 times ranked	1509 citing authors

#	Article	IF	Citations
1	Molecular Dynamics Simulation of a Silica Nanoparticle in Oligomeric Poly(methyl methacrylate): A Model System for Studying the Interphase Thickness in a Polymerâ€“Nanocomposite via Different Properties. Macromolecules, 2013, 46, 8680-8692.	4.8	108
2	Molecular dynamics simulation of diffusion and permeation of gases in polystyrene. Polymer, 2010, 51, 300-307.	3.8	83
3	How Thick is the Interphase in an Ultrathin Polymer Film? Coarse-Grained Molecular Dynamics Simulations of Polyamide-6,6 on Graphene. Journal of Physical Chemistry C, 2013, 117, 5249-5257.	3.1	69
4	Molecular Dynamics Simulation of Sorption of Gases in Polystyrene. Macromolecules, 2007, 40, 6413-6421.	4.8	66
5	Molecular dynamics simulation in the grand canonical ensemble. Journal of Computational Chemistry, 2007, 28, 1763-1773.	3.3	64
6	Molecular dynamics simulation of confined fluids in isosurface-isothermal-isobaric ensemble. Journal of Chemical Physics, 2008, 129, 194702.	3.0	64
7	Structure and Mobility of Nanoconfined Polyamide-6,6 Oligomers: Application of a Molecular Dynamics Technique with Constant Temperature, Surface Area, and Parallel Pressure. Journal of Physical Chemistry B, 2009, 113, 5568-5581.	2.6	62
8	A Refined All-Atom Model for the Ionic Liquid 1-n-Butyl 3-Methylimidazolium bis(Trifluoromethylsulfonyl)imide [bmim][Tf₂N]. Zeitschrift Fur Physikalische Chemie, 2007, 221, 1647-1662.	2.8	61
9	Molecular Dynamics Simulation of a Polyamide-66/Carbon Nanotube Nanocomposite. Journal of Physical Chemistry C, 2014, 118, 9841-9851.	3.1	61
10	Coarse-Grained Computer Simulation of Nanoconfined Polyamide-6,6. Macromolecules, 2011, 44, 3117-3128.	4.8	55
11	Molecular dynamics simulation with weak coupling to heat and material baths. Journal of Chemical Physics, 2010, 133, 084105.	3.0	47
12	Viscosity of Nanoconfined Polyamide-6,6 Oligomers: Atomistic Reverse Nonequilibrium Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2010, 114, 387-395.	2.6	47
13	Molecular Dynamics Simulation of Water Influence on Local Structure of Nanoconfined Polyamide-6,6. Journal of Physical Chemistry B, 2011, 115, 9720-9731.	2.6	47
14	Structure and Mobility of Poly(ethylene terephthalate): A Molecular Dynamics Simulation Study. Macromolecules, 2009, 42, 8241-8250.	4.8	44
15	Anisotropic heat transport in nanoconfined polyamide-6,6 oligomers: Atomistic reverse nonequilibrium molecular dynamics simulation. Journal of Chemical Physics, 2012, 136, 104901.	3.0	38
16	Sorption and diffusion of carbon dioxide and nitrogen in poly(methyl methacrylate). Journal of Chemical Physics, 2013, 139, 124902.	3.0	38
17	Local bond order parameters for accurate determination of crystal structures in two and three dimensions. Physical Chemistry Chemical Physics, 2018, 20, 27059-27068.	2.8	35
18	Reverse nonequilibrium molecular dynamics simulation of thermal conductivity in nanoconfined polyamide-6,6. Journal of Chemical Physics, 2011, 135, 064703.	3.0	32

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19	Mechanisms of Nucleation and Solidâ€“Solid-Phase Transitions in Triblock Janus Assemblies. Journal of Chemical Theory and Computation, 2021, 17, 1742-1754.	5.3	32
20	Structure, Dynamics, and Apparent Glass Transition of Stereoregular Poly(methyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 702 Td (methac	4.8	31
21	Thermal Conductivity of Polyamide-6,6/Carbon Nanotube Composites: Effects of Tube Diameter and Polymer Linkage between Tubes. Polymers, 2019, 11, 1465.	4.5	31
22	Ion-Pairing and Electrical Conductivity in the Ionic Liquid 1-n-Butyl-3-methylimidazolium Methylsulfate [Bmim][MeSO₄]: Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2017, 121, 7699-7708.	2.6	29
23	A Local Order Parameter-Based Method for Simulation of Free Energy Barriers in Crystal Nucleation. Journal of Chemical Theory and Computation, 2017, 13, 1307-1316.	5.3	28
24	Gaussian Charge Distributions for Incorporation of Electrostatic Interactions in Dissipative Particle Dynamics: Application to Self-Assembly of Surfactants. Journal of Chemical Theory and Computation, 2019, 15, 4197-4207.	5.3	28
25	Solidâ€“Liquid and Solidâ€“Solid Phase Diagrams of Self-Assembled Triblock Janus Nanoparticles from Solution. Journal of Physical Chemistry C, 2018, 122, 9235-9244.	3.1	27
26	Hydrogen bonding in water nanoconfined between graphene surfaces: a molecular dynamics simulation study. Journal of Nanoparticle Research, 2014, 16, 1.	1.9	26
27	Self-Assembly Mechanisms of Triblock Janus Particles. Journal of Chemical Theory and Computation, 2019, 15, 1345-1354.	5.3	25
28	How Alcoholic Disinfectants Affect Coronavirus Model Membranes: Membrane Fluidity, Permeability, and Disintegration. Journal of Physical Chemistry B, 2020, 124, 10374-10385.	2.6	22
29	Water permeability of poly(ethylene terephthalate): A grand canonical ensemble molecular dynamics simulation study. Journal of Chemical Physics, 2009, 131, 234904.	3.0	21
30	Structure and dynamics of stereo-regular poly(methyl-methacrylate) melts through atomistic molecular dynamics simulations. Soft Matter, 2018, 14, 1449-1464.	2.7	21
31	Self-Assembly of Model Triblock Janus Colloidal Particles in Two Dimensions. Journal of Chemical Theory and Computation, 2022, 18, 1870-1882.	5.3	16
32	Atomistic reverse nonequilibrium molecular dynamics simulation of the viscosity of ionic liquid 1-n-butyl 3-methylimidazolium bis(trifluoromethylsulfonyl)imide [bmim][Tf₂N]. Physical Chemistry Chemical Physics, 2018, 20, 21544-21551.	2.8	15
33	On the Equation of State for Quantum Systems. Journal of the Physical Society of Japan, 2000, 69, 1731-1734.	1.6	13
34	Local chemical potential and pressure tensor in inhomogeneous nanoconfined fluids. Journal of Chemical Physics, 2012, 137, 144702.	3.0	13
35	Adaptiveâ€numericalâ€bias metadynamics. Journal of Computational Chemistry, 2017, 38, 2721-2729.	3.3	13
36	Grand canonical ensemble molecular dynamics simulation of water solubility in polyamide-6,6. Physical Chemistry Chemical Physics, 2011, 13, 669-673.	2.8	12

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37	Coarse-grained molecular dynamics simulations of poly(ethylene terephthalate). Journal of Chemical Physics, 2020, 152, 114901.	3.0	12
38	Molecular dynamics simulation of liquidâ€“vapor phase equilibria in polar fluids. Chemical Physics Letters, 2009, 473, 66-71.	2.6	11
39	Prediction of the density for natural gas and liquefied natural gas mixtures. AICHE Journal, 2001, 47, 2585-2592.	3.6	9
40	Coarse Grained Molecular Dynamics Simulation of Nanoconfined Water. ChemPhysChem, 2013, 14, 1063-1070.	2.1	9
41	Molecular dynamics simulation of the diffusion of nanoconfined fluids. Journal of the Iranian Chemical Society, 2014, 11, 47-52.	2.2	8
42	Molecular Dynamics Simulation of the Ionic Liquid 1â€nâ€Butylâ€3â€Methylimidazolium Methylsulfate [Bmim][MeSO₄]: Interfacial Properties at the Silica and Vacuum Interfaces. ChemPhysChem, 2020, 21, 1134-1145.	2.1	8
43	Equation of state for mercury: revisited. Physics and Chemistry of Liquids, 2013, 51, 517-523.	1.2	6
44	A modified perturbed hard-sphere-chain equation of state for liquid refrigerant mixtures. Physics and Chemistry of Liquids, 2013, 51, 507-516.	1.2	6
45	Atomistic insights into structure, ion-pairing and ionic conductivity of 1-ethyl-3-methylimidazolium methylsulfate [Emim][MeSO4] ionic liquid from molecular dynamics simulation. Journal of Molecular Liquids, 2021, 331, 115803.	4.9	6
46	Solvation In Polymers. Challenges and Advances in Computational Chemistry and Physics, 2008, , 279-320.	0.6	6
47	How Ethanolic Disinfectants Disintegrate Coronavirus Model Membranes: A Dissipative Particle Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2022, 18, 2597-2615.	5.3	5
48	Nanoconfined polymers: modelling and simulation approaches. Molecular Simulation, 2015, 41, 367-381.	2.0	4
49	Rheology and morphology of no-slip sheared polymer nanocomposite under creep condition. Journal of Chemical Physics, 2015, 143, 034901.	3.0	3
50	Equation of State for Alkaline Earth Metals: Prediction from Boiling Point Constants. Journal of Chemical Engineering of Japan, 2004, 37, 871-874.	0.6	3
51	Temperature influence on the structure and dynamics of polymers at the interface: Atomistic molecular dynamics simulation of atactic polystyrene nanoconfined between graphene surfaces. Journal of Molecular Liquids, 2017, 244, 19-26.	4.9	2