Mohammad H Kowsari

List of Publications by Year
in descending order

22	601	759055 12	677027 22
papers	citations	h-index	g-index

22	22	22	724
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular dynamics simulation of imidazolium-based ionic liquids. I. Dynamics and diffusion coefficient. Journal of Chemical Physics, 2008, 129, 224508.	1.2	176
2	Simulations of structural and dynamic anisotropy in nano-confined water between parallel graphite plates. Journal of Chemical Physics, 2012, 137, 184703.	1.2	84
3	Molecular dynamics simulation of imidazolium-based ionic liquids. II. Transport coefficients. Journal of Chemical Physics, 2009, 130, 014703.	1.2	76
4	Molecular dynamics simulations of the structure and transport properties of tetra-butylphosphonium amino acid ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 8826.	1.3	49
5	Influence of Butyl Side Chain Elimination, Tail Amine Functional Addition, and C2 Methylation on the Dynamics and Transport Properties of Imidazolium-Based [Tf₂N^{â€“}] Ionic Liquids from Molecular Dynamics Simulations. Journal of Chemical & Engineering Data, 2015, 60, 551-560.	1.0	29
6	Tracing Dynamics, Self-Diffusion, and Nanoscale Structural Heterogeneity of Pure and Binary Mixtures of Ionic Liquid 1-Hexyl-2,3-dimethylimidazolium Bis(fluorosulfonyl)imide with Acetonitrile: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 10824-10838.	1.2	23
7	A new iron(III) complex of glycine derivative of amine-chloro substituted phenol ligand: Synthesis, characterization and catechol dioxygenase activity. Journal of Molecular Structure, 2012, 1029, 60-67.	1.8	22
8	Molecular Dynamics and ab Initio Studies of the Effects of Substituent Groups on the Thermodynamic Properties and Structure of Four Selected Imidazolium-Based [Tf₂N^{â€“}] Ionic Liquids. Journal of Chemical & Engineering Data, 2014, 59, 2834-2849.	1.0	20
9	A chloro bridged Cu(II)â€“Cu(II) complex of a new aminophenol ligand: Magnetostructural, radical decay kinetic studies, highly efficient and aerial alcohol oxidation. Polyhedron, 2012, 47, 94-103.	1.0	17
10	Capturing the effect of [PF₃(C₂F₅)₃]^{â^’}vs. [PF₆]^{â^’}, flexible anion vs. rigid, and scaled charge vs. unit on the transport properties of [bmim]⁺-based ionic liquids: a comparative MD study. Physical Chemistry Chemical Physics, 2018, 20, 13379-13393.	1.3	16
11	Atomistic insights into the thermodynamics, structure, and dynamics of ionic liquid 1-hexyl-3-methylimidazolium hexafluorophosphate via molecular dynamics study. Journal of Molecular Liquids, 2017, 246, 39-47.	2.3	14
12	Molecular dynamics study of congruent melting of the equimolar ionic liquid-benzene inclusion crystal [emim][NTf2]â€¢C6H6. Journal of Chemical Physics, 2010, 132, 044507.	1.2	12
13	Systematic evaluation and refinement of existing allâ€atom force fields for the simulation of liquid acetonitrile. Journal of Computational Chemistry, 2018, 39, 1843-1853.	1.5	12
14	Tracing Local Nanostructure of the Aqueous Solutions of the Biocompatible [Cho][Gly] Ionic Liquid: Importance of Hydrogen Bond Attraction between Like-Charged Ions. Journal of Physical Chemistry B, 2020, 124, 3770-3783.	1.2	12
15	Molecular Dynamics Insights into the Nanoscale Structural Organization and Local Interaction of Aqueous Solutions of Ionic Liquid 1-Butyl-3-methylimidazolium Nitrate. Journal of Physical Chemistry B, 2020, 124, 6972-6985.	1.2	9
16	Understanding the dynamics, self-diffusion, and microscopic structure of hydrogen inside the nanoporous Li-LSX zeolite. Microporous and Mesoporous Materials, 2017, 240, 39-49.	2.2	8
17	Molecular dynamics simulations of nano-confined methanol and methanol-water mixtures between infinite graphite plates: Structure and dynamics. Journal of Chemical Physics, 2019, 150, 144510.	1.2	6
18	Tracing Experimentally Compatible Dynamical and Structural Behavior of Atmospheric N2/O2Binary Mixtures within Nanoporous Liâ€“LSX Zeolite: New Insights to Influence of Extra-Framework Cations by MD Simulations. Journal of Physical Chemistry C, 2017, 121, 1770-1780.	1.5	5

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19	Fine probing the effect of replacing [PF₆]^{â˜’} with [PF₃(C₂F₅)₃]^{â˜’} on the local structure and nanoscale organization of [bmim]⁺-based ionic liquids using MD simulation. Physical Chemistry Chemical Physics, 2019, 21, 3195-3210.	1.3	4
20	Single-component structural correlation and self-diffusion of N 2 and O 2 through nanopores of Li-LSX zeolite: The role of temperature, loading, and Li-III cations. Microporous and Mesoporous Materials, 2018, 264, 181-189.	2.2	3
21	The possibility of cadmium extraction to the ionic liquid 1-hexyl-3-methylimidazolium hexafluorophosphate in the presence of hydrochloric acid: a molecular dynamics study of the waterâ€“IL interface. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	3
22	Tracing the origin of heterogeneities in the local structure and very sluggish dynamics of [Cho][Gly] ionic liquid confined between rutile and graphite slit nanopores: A MD study. Journal of Chemical Physics, 2022, 156, .	1.2	1