Saied Yeganegi

List of Publications by Year in Descending Order

44 papers	571 citations	12 h-index	22 g-index
46 ext. papers	648 ext. citations	3.2 avg, IF	4.32 L-index

#	Paper	IF	Citations
44	The Diffusion of Light Gases through Polyvinyl Butyral: Molecular Hydrogen, Helium, and Neon. *Journal of Molecular Liquids*, **2021**, 345, 118245	6	
43	Molecular simulations of the adsorption and separation of hydrogen sulfide, carbon dioxide, methane, and nitrogen and their binary mixtures (HS/CH), (CO/CH) on NUM-3a metal-organic frameworks. *Journal of Molecular Modeling*, **2021**, 27, 133	2	2
42	Computational study of the effect of functionalization on natural gas components separation and adsorption in NUM-3a MOF. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107731	2.8	4
41	H2S separation from biogas by adsorption on functionalized MIL-47-X (X = OH and OCH3): A simulation study. *Applied Surface Science*, **2019**, 479, 1006-1013	6.7	11
40	Adsorption of 5-Fluorouracil and Thioguanine drugs into ZIF-1, ZIF-3 and ZIF-6 by simulation methods. *Materials Science and Engineering C*, **2019**, 97, 461-466	8.3	12
39	Computational study of halogen-free Boron based dicationic ionic liquids of [bis-Mim][BMB] and [bis-Mim][BScB]. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 210, 181-192	4.4	2
38	DFT study of structures and hydrogen bonds of imidazolium based halogen-free boron containing dicationic ionic liquids. *Journal of Molecular Liquids*, **2018**, 256, 330-343	6	15
37	Molecular simulations of adsorption and separation of ethylene/ethane and propylene/propane mixtures on Ni2(dobdc) and Ni2(m-dobdc) metal-organic frameworks. *Molecular Simulation*, **2018**, 44, 389-395	2	8
36	Adsorption of propylene, propane, ethylene and ethane in an isoreticular series of MOF-74 structures. *Adsorption*, **2017**, 23, 507-514	2.6	4
35	Molecular simulations of adsorption and separation of acetylene and methane and their binary mixture on MOF-5, HKUST-1 and MOF-505 metal–organic frameworks. *Molecular Simulation*, **2017**, 43, 260-266	2	7
34	Adsorption of 5-fluorouracil, hydroxyurea and mercaptopurine drugs on zeolitic imidazolate frameworks (ZIF-7, ZIF-8 and ZIF-9). *Microporous and Mesoporous Materials*, **2017**, 252, 167-172	5.3	30
33	MD study of structure and dynamic properties of the 1-n-alkyl-3-methylimidazolium tris(perfluoroalkyl)trifluorophosphate ionic liquids. *Journal of Molecular Liquids*, **2017**, 244, 77-84	6	7
32	Molecular Dynamics Simulations of Amide Functionalized Imidazolium Bis(trifluoromethanesulfonyl)imide Dicationic Ionic Liquids. *Journal of Physical Chemistry B*, **2017**, 121, 7455-7463	3.4	3
31	Molecular dynamic simulation study of molten cesium. *Journal of the Serbian Chemical Society*, **2017**, 82, 681-694	0.9	1
30	Hydrogen physisorption and selectivity in single-walled silicon carbon nanotubes: a grand canonical Monte-Carlo study. *Journal of the Iranian Chemical Society*, **2016**, 13, 207-220	2	9
29	Multiscale Computational Study on the Adsorption and Separation of CO /CH and CO /H on Li -Doped Mixed-Ligand Metal-Organic Framework Zn (NDC) (diPyNI). *ChemPhysChem*, **2016**, 17, 4124-4133	3.2	16
28	Adsorption of hydrogen and methane on intrinsic and alkali metal cations-doped Zn2(NDC)2(diPyTz) metal–organic framework using GCMC simulations. *Adsorption*, **2016**, 22, 277-285	2.6	6

27	Simulation of methane adsorption and diffusion in a carbon nanotube channel. *Chemical Engineering Science*, **2016**, 140, 62-70	4.4	20
26	Molecular simulation study on the adsorption and separation of acidic gases in a model nanoporous carbon. *Chemical Engineering Science*, **2014**, 117, 426-435	4.4	24
25	A Differential Scanning Calorimetry and Theoretical Study on the Isomerization of trans-[Co(cyclam)(ONO)2]X (X = PF6, ClO4). *European Journal of Inorganic Chemistry*, **2014**, 2014, 4788-4802	2.3	5
24	Ab initio study of hydrogen adsorption on Zn2(NDC)2(diPyTz) metal-organic framework decorated with alkali and alkaline earth metal cations. *International Journal of Hydrogen Energy*, **2014**, 39, 14008-14017	6.7	3
23	A theoretical investigation on the regioselectivity of the intramolecular hetero Diels-Alder and 1,3-dipolar cycloaddition of 2-vinyloxybenzaldehyde derivatives. *Journal of the Serbian Chemical Society*, **2014**, 79, 911-924	0.9	8
22	Study of thermodynamic properties of imidazolium-based ionic liquids and investigation of the alkyl chain length effect by molecular dynamics simulation. *Molecular Simulation*, **2013**, 39, 1070-1078	2	18
21	Methane adsorption and diffusion in a model nanoporous carbon: an atomistic simulation study. *Adsorption*, **2013**, 19, 979-987	2.6	12
20	Thermal diffusion factor of Stockmayer mixtures: A non-equilibrium molecular dynamic study. *Chemical Physics*, **2013**, 415, 119-123	2.3	2
19	DFT Study of the Geometrical and Electronic Structures of Geminal Dicationic Ionic Liquids 1,3-Bis[3-methylimidazolium-1-yl]hexane Halides. *Journal of the Chinese Chemical Society*, **2013**, 60, 551-558	1.5	8
18	First-principles vdW-DF investigation on the interaction between the oxazepam molecule and C fullerene. *Journal of Molecular Modeling*, **2013**, 19, 1929-36	2	12
17	Molecular dynamic simulation of dicationic ionic liquids: effects of anions and alkyl chain length on liquid structure and diffusion. *Journal of Physical Chemistry B*, **2012**, 116, 11517-26	3.4	70
16	Experimental and theoretical approaches to [1,5]-prototropic generation of an azomethine ylide and a 1,3-dipolar cycloaddition for novel spiropyrrolidine oxindoles synthesis. *Journal of Molecular Structure*, **2012**, 1030, 168-176	3.4	24
15	Hydrogen adsorption capacities of multi-walled boron nitride nanotubes and nanotube arrays: a grand canonical Monte Carlo study. *Journal of Molecular Modeling*, **2012**, 18, 2981-91	2	16
14	Phosphonate monoesters as carboxylate-like linkers for metal organic frameworks. *Journal of the American Chemical Society*, **2011**, 133, 20048-51	16.4	81
13	An experimental and theoretical investigation of the regio- and stereoselectivity of the polar [3+2] cycloaddition of azomethine ylides to nitrostyrenes. *Tetrahedron*, **2011**, 67, 1589-1597	2.4	57
12	Ab initio interaction potential of methane and nitrogen. *Chemical Physics Letters*, **2009**, 467, 237-242	2.5	23
11	Thermal Diffusion Factor of Binary Mixtures of Square Well Fluids. *Journal of the Physical Society of Japan*, **2008**, 77, 074604	1.5	
10	Cyclic voltammetric and computational study of a 4-bromophenyl monolayer on a glassy carbon electrode. *Monatshefte F Chemie*, **2008**, 139, 781-787	1.4	1

9	Thermal diffusion factor of model 2CLJD mixtures from non-equilibrium molecular dynamics. *Chemical Physics Letters*, **2008**, 451, 209-212	2.5	2
8	Theoretical study of energetics and mechanisms of cis–trans interconversion of 1,3-diphenyltriazene. *Computational and Theoretical Chemistry*, **2008**, 867, 47-52		1
7	Comparison of Efficiency Equilibrium and Non-Equilibrium Molecular Dynamics Calculations of Thermal Diffusion Factor. *Journal of the Physical Society of Japan*, **2007**, 76, 044601	1.5	2
6	The effect of corrugation of pore wall on the thermal diffusion in nanopores by molecular dynamics simulations. *Chemical Physics*, **2007**, 333, 69-76	2.3	7
5	Non-equilibrium molecular dynamics calculation of thermal diffusion factor in binary mixtures of hard spheres. *Fluid Phase Equilibria*, **2006**, 243, 161-165	2.5	10
4	Dependence of thermal diffusion factor of binary mixtures to the thermodynamic state by NEMD simulation. *Chemical Physics*, **2005**, 318, 171-179	2.3	5
3	Temperature Dependence of Thermal Diffusion Factor for Isotopic Binary Mixtures by Non-Equilibrium Molecular Dynamics Simulation. *Journal of the Physical Society of Japan*, **2003**, 72, 2260-2264	1.5	3
2	Nonequilibrium Molecular Dynamics Study of Thermal Diffusion Behavior of the MMSV Potential Model for Hydrogen. *Journal of the Physical Society of Japan*, **2001**, 70, 3261-3267	1.5	5
1	On the Sensitivity of Thermal Diffusion to the Intermolecular Pair Potential. *Journal of the Physical Society of Japan*, **2000**, 69, 1389-1393	1.5	12