

# Saied Yeganegi

## List of Publications by Citations

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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.

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	Phosphonate monoesters as carboxylate-like linkers for metal organic frameworks. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 20048-51	16.4	81
43	Molecular dynamic simulation of dicationic ionic liquids: effects of anions and alkyl chain length on liquid structure and diffusion. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 11517-26	3.4	70
42	An experimental and theoretical investigation of the regio- and stereoselectivity of the polar [3+2] cycloaddition of azomethine ylides to nitrostyrenes. <i>Tetrahedron</i> , <b>2011</b> , 67, 1589-1597	2.4	57
41	Adsorption of 5-fluorouracil, hydroxyurea and mercaptopurine drugs on zeolitic imidazolate frameworks (ZIF-7, ZIF-8 and ZIF-9). <i>Microporous and Mesoporous Materials</i> , <b>2017</b> , 252, 167-172	5.3	30
40	Molecular simulation study on the adsorption and separation of acidic gases in a model nanoporous carbon. <i>Chemical Engineering Science</i> , <b>2014</b> , 117, 426-435	4.4	24
39	Experimental and theoretical approaches to [1,5]-prototropic generation of an azomethine ylide and a 1,3-dipolar cycloaddition for novel spiropyrrolidine oxindoles synthesis. <i>Journal of Molecular Structure</i> , <b>2012</b> , 1030, 168-176	3.4	24
38	Ab initio interaction potential of methane and nitrogen. <i>Chemical Physics Letters</i> , <b>2009</b> , 467, 237-242	2.5	23
37	Simulation of methane adsorption and diffusion in a carbon nanotube channel. <i>Chemical Engineering Science</i> , <b>2016</b> , 140, 62-70	4.4	20
36	Study of thermodynamic properties of imidazolium-based ionic liquids and investigation of the alkyl chain length effect by molecular dynamics simulation. <i>Molecular Simulation</i> , <b>2013</b> , 39, 1070-1078	2	18
35	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). <i>ChemPhysChem</i> , <b>2016</b> , 17, 4124-4133 <sup>3,2</sup>	3.2	16
34	Hydrogen adsorption capacities of multi-walled boron nitride nanotubes and nanotube arrays: a grand canonical Monte Carlo study. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 2981-91	2	16
33	DFT study of structures and hydrogen bonds of imidazolium based halogen-free boron containing dicationic ionic liquids. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 256, 330-343	6	15
32	Methane adsorption and diffusion in a model nanoporous carbon: an atomistic simulation study. <i>Adsorption</i> , <b>2013</b> , 19, 979-987	2.6	12
31	First-principles vdW-DF investigation on the interaction between the oxazepam molecule and C <sub>60</sub> fullerene. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 1929-36	2	12
30	On the Sensitivity of Thermal Diffusion to the Intermolecular Pair Potential. <i>Journal of the Physical Society of Japan</i> , <b>2000</b> , 69, 1389-1393	1.5	12
29	Adsorption of 5-Fluorouracil and Thioguanine drugs into ZIF-1, ZIF-3 and ZIF-6 by simulation methods. <i>Materials Science and Engineering C</i> , <b>2019</b> , 97, 461-466	8.3	12
28	H <sub>2</sub> S separation from biogas by adsorption on functionalized MIL-47-X (X = OH and [DCH <sub>3</sub> ): A simulation study. <i>Applied Surface Science</i> , <b>2019</b> , 479, 1006-1013	6.7	11

27	Non-equilibrium molecular dynamics calculation of thermal diffusion factor in binary mixtures of hard spheres. <i>Fluid Phase Equilibria</i> , <b>2006</b> , 243, 161-165	2.5	10
26	Hydrogen physisorption and selectivity in single-walled silicon carbon nanotubes: a grand canonical Monte-Carlo study. <i>Journal of the Iranian Chemical Society</i> , <b>2016</b> , 13, 207-220	2	9
25	Molecular simulations of adsorption and separation of ethylene/ethane and propylene/propane mixtures on Ni <sub>2</sub> (dobdc) and Ni <sub>2</sub> (m-dobdc) metal-organic frameworks. <i>Molecular Simulation</i> , <b>2018</b> , 44, 389-395	2	8
24	A theoretical investigation on the regioselectivity of the intramolecular hetero Diels-Alder and 1,3-dipolar cycloaddition of 2-vinyloxybenzaldehyde derivatives. <i>Journal of the Serbian Chemical Society</i> , <b>2014</b> , 79, 911-924	0.9	8
23	DFT Study of the Geometrical and Electronic Structures of Geminal Dicationic Ionic Liquids 1,3-Bis[3-methylimidazolium-1-yl]hexane Halides. <i>Journal of the Chinese Chemical Society</i> , <b>2013</b> , 60, 551-558	1.5	8
22	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. <i>Molecular Simulation</i> , <b>2017</b> , 43, 260-266	2	7
21	MD study of structure and dynamic properties of the 1-n-alkyl-3-methylimidazolium tris(perfluoroalkyl)trifluorophosphate ionic liquids. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 244, 77-84	6	7
20	The effect of corrugation of pore wall on the thermal diffusion in nanopores by molecular dynamics simulations. <i>Chemical Physics</i> , <b>2007</b> , 333, 69-76	2.3	7
19	Adsorption of hydrogen and methane on intrinsic and alkali metal cations-doped Zn <sub>2</sub> (NDC)2(diPyTz) metal-organic framework using GCMC simulations. <i>Adsorption</i> , <b>2016</b> , 22, 277-285	2.6	6
18	A Differential Scanning Calorimetry and Theoretical Study on the Isomerization of trans-[Co(cyclam)(ONO)2]X (X = PF <sub>6</sub> <sup>-</sup> , ClO <sub>4</sub> <sup>-</sup> ). <i>European Journal of Inorganic Chemistry</i> , <b>2014</b> , 2014, 4788-4802	2.3	5
17	Dependence of thermal diffusion factor of binary mixtures to the thermodynamic state by NEMD simulation. <i>Chemical Physics</i> , <b>2005</b> , 318, 171-179	2.3	5
16	Nonequilibrium Molecular Dynamics Study of Thermal Diffusion Behavior of the MMSV Potential Model for Hydrogen. <i>Journal of the Physical Society of Japan</i> , <b>2001</b> , 70, 3261-3267	1.5	5
15	Adsorption of propylene, propane, ethylene and ethane in an isorecticular series of MOF-74 structures. <i>Adsorption</i> , <b>2017</b> , 23, 507-514	2.6	4
14	Computational study of the effect of functionalization on natural gas components separation and adsorption in NUM-3a MOF. <i>Journal of Molecular Graphics and Modelling</i> , <b>2020</b> , 101, 107731	2.8	4
13	Ab initio study of hydrogen adsorption on Zn <sub>2</sub> (NDC)2(diPyTz) metal-organic framework decorated with alkali and alkaline earth metal cations. <i>International Journal of Hydrogen Energy</i> , <b>2014</b> , 39, 14008-14017	6.7	3
12	Molecular Dynamics Simulations of Amide Functionalized Imidazolium Bis(trifluoromethanesulfonyl)imide Dicationic Ionic Liquids. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 7455-7463	3.4	3
11	Temperature Dependence of Thermal Diffusion Factor for Isotopic Binary Mixtures by Non-Equilibrium Molecular Dynamics Simulation. <i>Journal of the Physical Society of Japan</i> , <b>2003</b> , 72, 2260-2264	1.5	3
10	Thermal diffusion factor of Stockmayer mixtures: A non-equilibrium molecular dynamic study. <i>Chemical Physics</i> , <b>2013</b> , 415, 119-123	2.3	2

9	Comparison of Efficiency Equilibrium and Non-Equilibrium Molecular Dynamics Calculations of Thermal Diffusion Factor. <i>Journal of the Physical Society of Japan</i> , <b>2007</b> , 76, 044601	1.5	2
8	Thermal diffusion factor of model 2CLJD mixtures from non-equilibrium molecular dynamics. <i>Chemical Physics Letters</i> , <b>2008</b> , 451, 209-212	2.5	2
7	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. <i>Journal of Molecular Modeling</i> , <b>2021</b> , 27, 133	2	2
6	Computational study of halogen-free Boron based dicationic ionic liquids of [bis-Mim][BMB] and [bis-Mim][BScB]. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2019</b> , 210, 181-192	4.4	2
5	Cyclic voltammetric and computational study of a 4-bromophenyl monolayer on a glassy carbon electrode. <i>Monatshefte für Chemie</i> , <b>2008</b> , 139, 781-787	1.4	1
4	Theoretical study of energetics and mechanisms of cis-trans interconversion of 1,3-diphenyltriazene. <i>Computational and Theoretical Chemistry</i> , <b>2008</b> , 867, 47-52		1
3	Molecular dynamic simulation study of molten cesium. <i>Journal of the Serbian Chemical Society</i> , <b>2017</b> , 82, 681-694	0.9	1
2	Thermal Diffusion Factor of Binary Mixtures of Square Well Fluids. <i>Journal of the Physical Society of Japan</i> , <b>2008</b> , 77, 074604	1.5	
1	The Diffusion of Light Gases through Polyvinyl Butyral: Molecular Hydrogen, Helium, and Neon. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 345, 118245	6	