Xuanjun Wu

List of Publications by Year
in descending order

13	259	1039406 9	1125271 13
papers	citations	h-index	g-index

14	14	14	347
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Force field for ZIF-8 flexible frameworks: atomistic simulation of adsorption, diffusion of pure gases as CH₄, H₂, CO₂ and N₂. RSC Advances, 2014, 4, 16503-16511.	1.7	64
2	Understanding Quantitative Relationship between Methane Storage Capacities and Characteristic Properties of Metalâ€“Organic Frameworks Based on Machine Learning. Journal of Physical Chemistry C, 2019, 123, 8550-8559.	1.5	49
3	Ultrahigh hydrogen storage capacity of novel porous aromatic frameworks. Journal of Materials Chemistry A, 2015, 3, 10724-10729.	5.2	23
4	Computational design of tetrazolate-based metalâ€“organic frameworks for CH₄ storage. Physical Chemistry Chemical Physics, 2018, 20, 30150-30158.	1.3	18
5	High-throughput computational screening of metalâ€“organic frameworks with topological diversity for hexane isomer separations. Physical Chemistry Chemical Physics, 2019, 21, 8508-8516.	1.3	18
6	Hydrogen storage metal-organic framework classification models based on crystal graph convolutional neural networks. Chemical Engineering Science, 2022, 259, 117813.	1.9	16
7	Computational screening of metal-organic frameworks with open copper sites for hydrogen purification. International Journal of Hydrogen Energy, 2020, 45, 27320-27330.	3.8	15
8	Revealing enhancement mechanism of volumetric hydrogen storage capacity of nano-porous frameworks by molecular simulation. Chemical Engineering Science, 2020, 226, 115837.	1.9	13
9	Highâ€throughput computational screening of porous polymer networks for natural gas sweetening based on a neural network. AIChE Journal, 2022, 68, e17433.	1.8	11
10	Effect of an acetylene bond on hydrogen adsorption in diamond-like carbon allotropes: from first principles to atomic simulation. Physical Chemistry Chemical Physics, 2017, 19, 9261-9269.	1.3	9
11	Preparation and characterization of polylactide/montmorillonite nanocomposites. Journal Wuhan University of Technology, Materials Science Edition, 2009, 24, 562-565.	0.4	8
12	High-throughput Screening of Real Metal-organic Frameworks for Adsorption Separation of C4 Olefins. Acta Chimica Sinica, 2021, 79, 520.	0.5	8
13	Ionic liquid screening for desulfurization of coke oven gas based on COSMO-SAC model and process simulation. Chemical Engineering Research and Design, 2021, 176, 146-161.	2.7	7