# Xuanjun Wu

List of Publications by Year
in descending order

| 13 papers | 259 citations | 1039406<br>9 h-index | 1125271<br>13 g-index |
|---|---|---|---|
| 14 all docs | 14 docs citations | 14 times ranked | 347 citing authors |

| # | Article | IF | Citations |
|---|---------|----|-----------| 
| 1 | High‐throughput computational screening of porous polymer networks for natural gas sweetening based on a neural network. AICHE Journal, 2022, 68, e17433. | 1.8 | 11 |
| 2 | Hydrogen storage metal-organic framework classification models based on crystal graph convolutional neural networks. Chemical Engineering Science, 2022, 259, 117813. | 1.9 | 16 |
| 3 | High-throughput Screening of Real Metal-organic Frameworks for Adsorption Separation of C4 Olefins. Acta Chimica Sinica, 2021, 79, 520. | 0.5 | 8 |
| 4 | 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 |
| 5 | 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 |
| 6 | Revealing enhancement mechanism of volumetric hydrogen storage capacity of nano-porous frameworks by molecular simulation. Chemical Engineering Science, 2020, 226, 115837. | 1.9 | 13 |
| 7 | Understanding Quantitative Relationship between Methane Storage Capacities and Characteristic Properties of Metal–Organic Frameworks Based on Machine Learning. Journal of Physical Chemistry C, 2019, 123, 8550-8559. | 1.5 | 49 |
| 8 | High-throughput computational screening of metal–organic frameworks with topological diversity for hexane isomer separations. Physical Chemistry Chemical Physics, 2019, 21, 8508-8516. | 1.3 | 18 |
| 9 | Computational design of tetrazolate-based metal–organic frameworks for $CH_4$ storage. Physical Chemistry Chemical Physics, 2018, 20, 30150-30158. | 1.3 | 18 |
| 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 | Ultrahigh hydrogen storage capacity of novel porous aromatic frameworks. Journal of Materials Chemistry A, 2015, 3, 10724-10729. | 5.2 | 23 |
| 12 | Force field for ZIF-8 flexible frameworks: atomistic simulation of adsorption, diffusion of pure gases as $CH_4$, $H_2$, $CO_2$ and $N_2$. RSC Advances, 2014, 4, 16503-16511. | 1.7 | 64 |
| 13 | Preparation and characterization of polylactide/montmorillonite nanocomposites. Journal Wuhan University of Technology, Materials Science Edition, 2009, 24, 562-565. | 0.4 | 8 |