a. Methane storage

b. Carbon capture

c. Natural gas upgrade

Data: 137,953 hMOFs
Simulation: 500 GCMC cycles
Metric: adsorption capacity

Data: 169,898 ZIF Models
Simulation: Materials studio
Metric: porosity and stability

Data: 137,953 Wilmer's hMOFs
Simulation: Zeo++
Metric: PLD between 3 Å and 4 Å

Data: 7,000 best hMOFs
Simulation: 2,500 GCMC cycles
Metric: adsorption capacity

Data: 83,070 hZIFs Simulation: GCMC

Data: 17,257 hMOFs
Simulation: MC and MD
Metric: over Robeson's bound

Data: 350 best hMOFs
Simulation: 12,500 GCMC cycles
Metric: adsorption capacity

Data: 7,959 hZIFs
Simulation: multi-component GCMC
Metric: working capacity, selectivity
and adsorbent performance score

Metric: selectivity at infinite dilution

Data: 24 hMOFs
Simulation: mixture GCMC and MD
Metric: permeation of mixture at
working pressure and temperature

Best materials
Comparison to experiments
Structure-property relationship

Promising Top 49 hydrophobic ZIF materials for CO₂/N₂ separation

5 Best MOF materials for CO₂/N₂/CH₄ ternary separation

Wilmer *et al.*, 2012

Yang et al., 2020

Qiao et al., 2016