Molecular Simulation for Adsorption and Separation of CH₄/H₂ in Zeolitic Imidazolate Frameworks

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S1. Comparison of absolute isotherms on ZIF-8 and MOF-5

Figure S1 Comparison of the simulated and experimental⁶ absolute isotherms on ZIF-8 and MOF-5 at 300K for (a) CH₄ and (b) H₂

S2. Isostatic heats of adsorption vs. pressures

Figure S2 Isostatic heats of adsorption vs. pressures, (a) CH_4 , and (b) H_2 (the adsorbate-adsorbent part)

S3. Density distribution profiles on ZIF-67

Figure S3 Density distribution profiles on ZIF-67 for (a) CH₄, and (b) H₂