

Electronic Supplementary Information

Upgrade of natural gas in *rho* zeolite-like metal-organic framework and effect of water: A computational study

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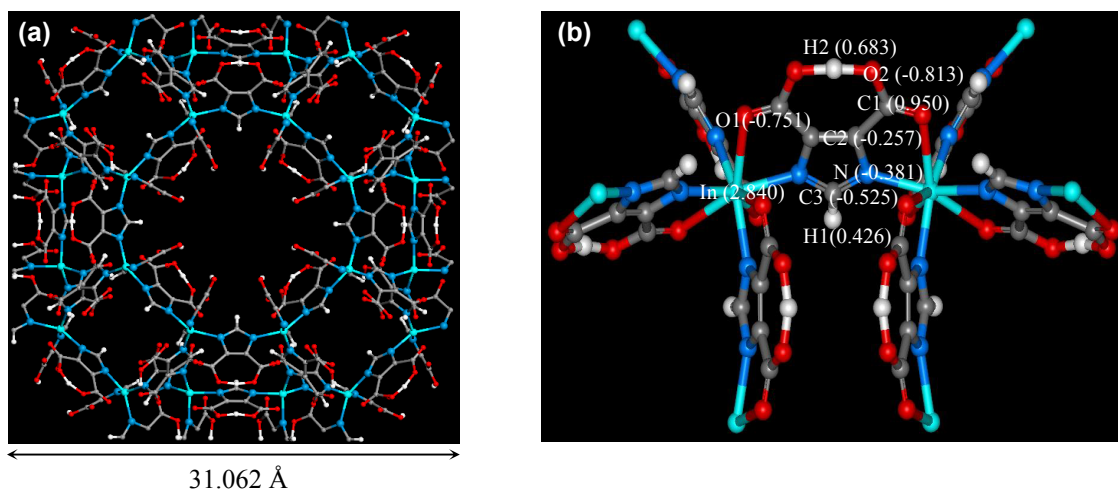


Figure S1. (a) A unit cell of *rho*-ZMOF (b) Atomic charges in a fragmental cluster of *rho*-ZMOF. The extraframework ions are not shown. Color code: In, cyan; N, blue; C, grey; O, red; and H, white.

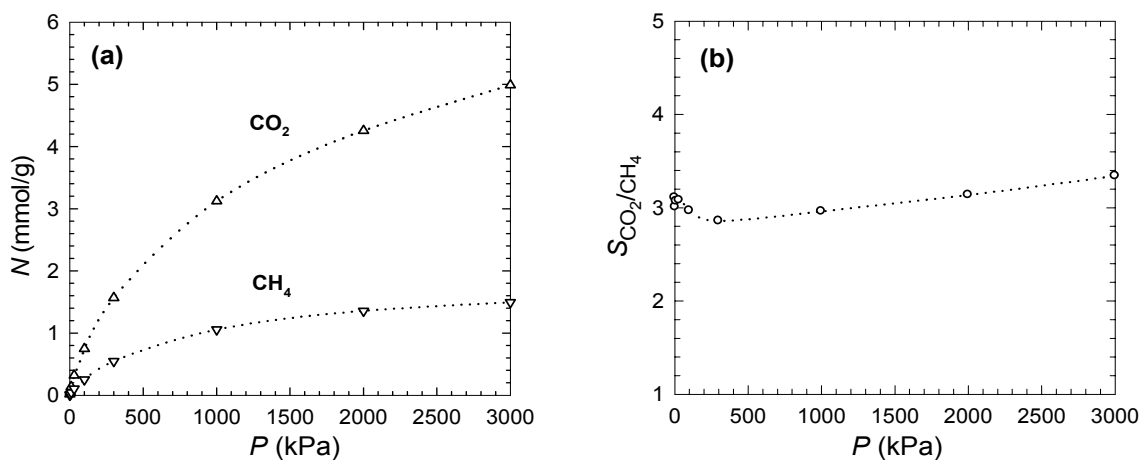


Figure S2. (a) Adsorption isotherm (b) Selectivity for CO₂/CH₄ mixture. The charges on framework and extraframework ions were switched off.