

Supplementary Information For
**Adsorption and Transport of CH₄, CO₂, H₂ Mixtures in a Bio-MOF Material from
Molecular Simulations**

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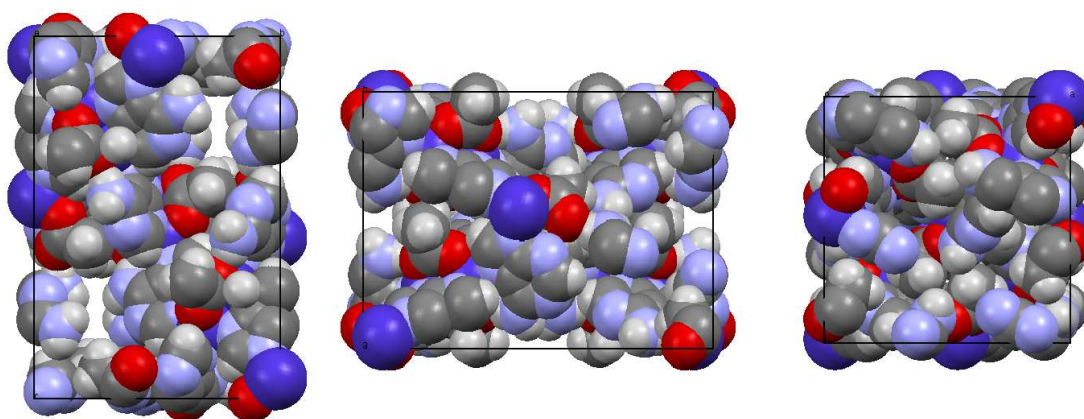
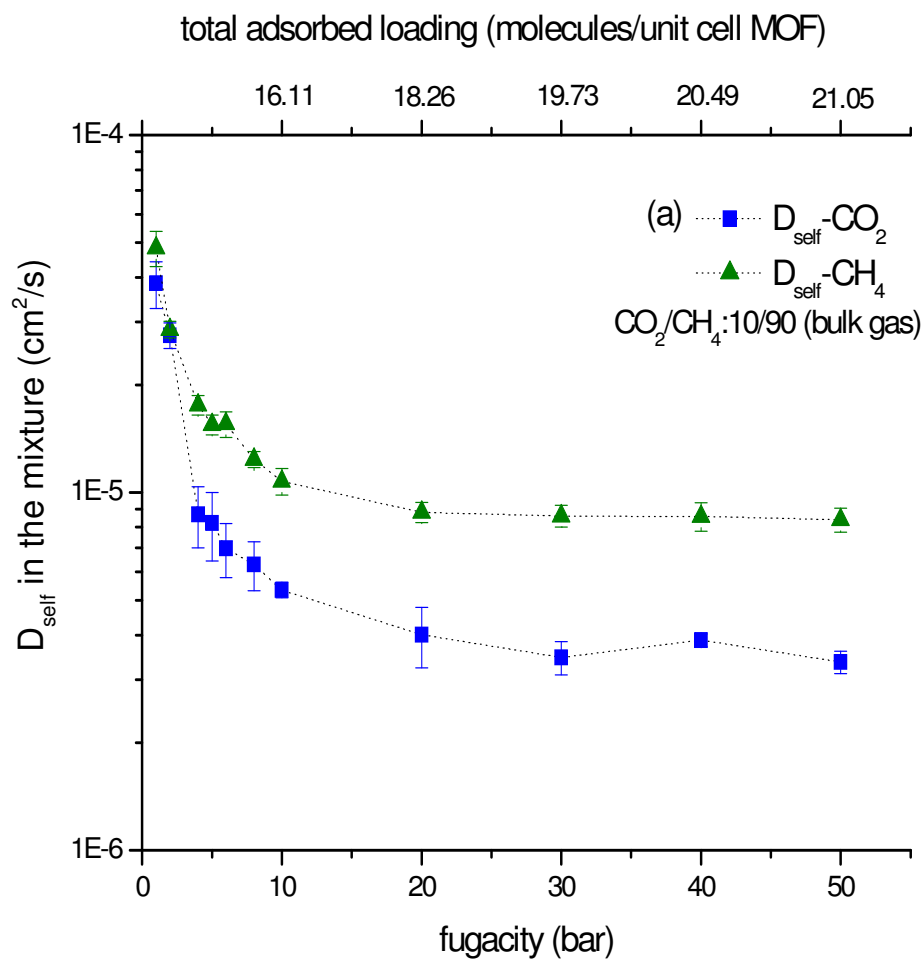


Figure S1. Unit cell structure of bio-MOF-11 in *x*, *y*, and *z* directions (from left to right).
Red:oxygen, blue:cobalt, purple:nitrogen, grey:carbon, white:hydrogen.



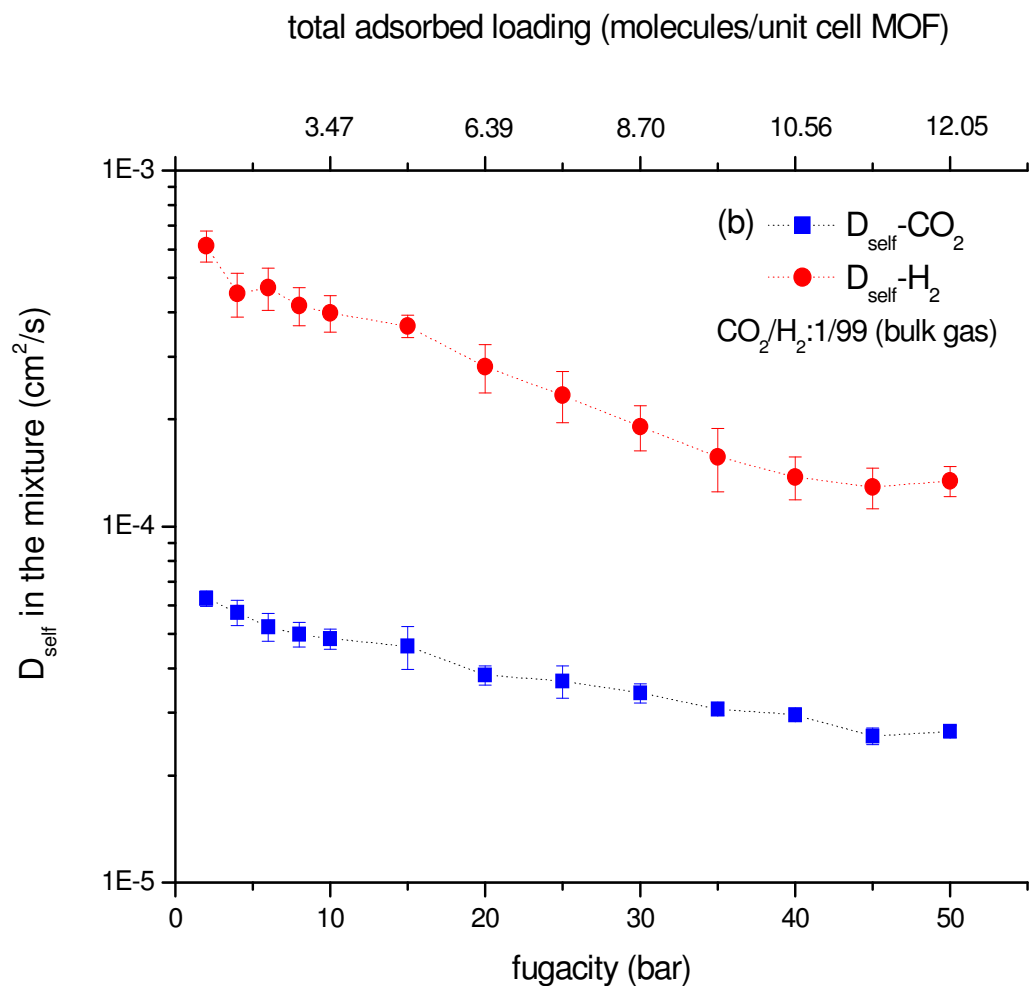
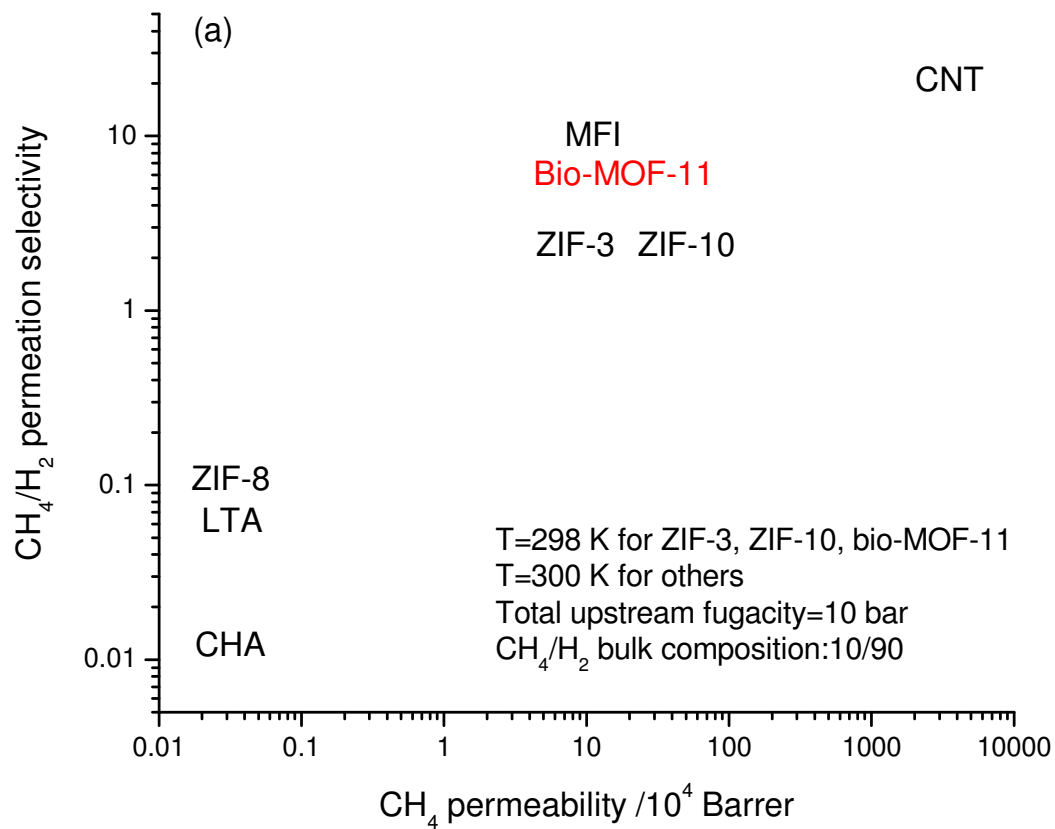
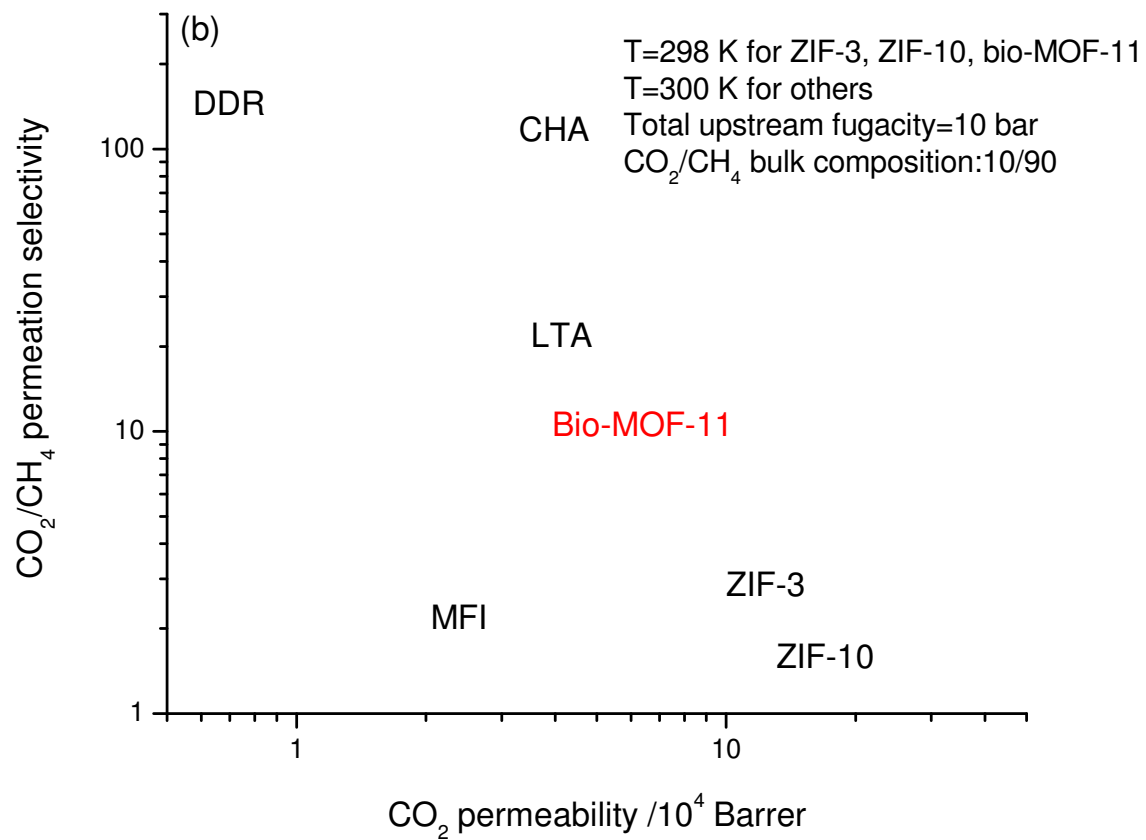


Figure S2. Self diffusivities of gas species in their binary mixtures in bio-MOF-11 for a) CO_2/CH_4 b) CO_2/H_2 at 298 K as functions of fugacity and total adsorbed loading. The bulk mixtures are $\text{CO}_2/\text{CH}_4:10/90$ and $\text{CO}_2/\text{H}_2:1/99$.





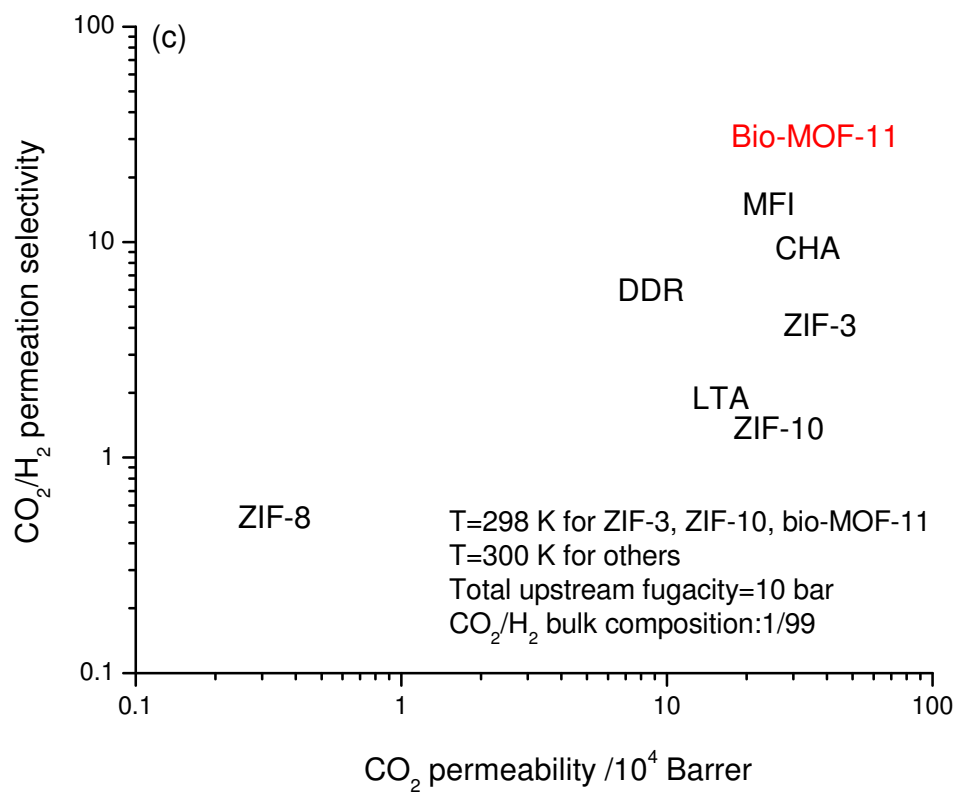


Figure S3. Predicted gas permeabilities and selectivities of bio-MOF-11 membranes for a)CH₄/H₂ b)CO₂/CH₄ and c)CO₂/H₂ mixtures. Data for other membranes are taken from references 26 and 52.