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High-throughput computational screening of metal-organic framework membranes for upgrading of natural gas

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ABSTRACT: We report a computational study to screen 4764 computation-ready experimental metal-organic frameworks (CoRE-MOF) for the membrane separation of a ternary gas mixture ($CO_2/N_2/CH_4$) at 298 K and 10 bar. Combining Monte Carlo and molecular dynamics simulations, the adsorption, diffusion and permeation of the gas mixture are predicted. The structure-performance relationships are established between the geometrical descriptors of MOFs (pore liming diameter, density, void fraction and volumetric surface area) and the evaluation criteria of membrane performance (permeability and permselectivity). Furthermore, principal component analysis is used to assess the interrelationships among the descriptors, then multiple linear regression is applied to quantitatively determine the respective effects of descriptors on performance. In addition, decision tree modelling is adopted to define a clear effective path for screening. Finally, seven best MOF membranes are identified for single-step separation of both CO_2 and N_2 from CH_4. The microscopic insights and structure-performance relationships from this computational study can facilitate the development of new MOF membranes for the upgrading of natural gas.

Graphical abstract:

A computational study is reported to screen 4764 computation-ready experimental MOFs for membrane separation of CH_4 from a ternary $CO_2/N_2/CH_4$ mixture.

KEYWORDS: metal-organic frameworks, membrane separation, natural gas, computational screening, molecular simulation

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