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Computational-aided development of MOF-based Mixed Matrix Membranes for molecular separation

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Mixed matrix membranes (MMMs) incorporating MOFs into polymeric matrices show promising properties for several key gas separation processes. Understanding of the MOF/polymer interface and gas transport through the MMMs is of utmost importance. Here, we selected a series of MOFs as fillers in conjunction with both rigid and flexible polymers and we deployed our in-house computational strategy to construct MOF/Polymer atomistic models and assess their thermodynamic and dynamic adsorption properties. This computational screening revealed that the distinct characteristic of polymer backbones and MOF surfaces results in different interfacial pore structuring. We evidenced that not only size but also shape of the interfacial pore region has eminent effects on the gas transport properties of the MMMs with respect to a selected range of molecules. This conclusion is an important step toward the rational design of MMMs with the optimal interfacial pore size/shape to achieve the best performance for molecular separation. This computational strategy has been also applied recently to explore the shaping of MOFs with the selection of the appropriate polymers of crucial importance in diverse industrial applications including CO2 capture.

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