How MOF/Polymer Interfacial void shape/size affect the gas permeability of Mixed Matrix Membranes

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Abstract

Mixed matrix membranes (MMMs) incorporating Metal-organic frameworks (MOF) into polymeric matrices show promising properties for several industrial applications, such as gas separation, water desalination and pervaporation among others. Especially in the field of gas separation, MMMs have attracted a great attention owing to their potential for merging the processability of polymers and the excellent selectivity of MOF materials. Therefore, understanding gas transport through the MMMs is of significant importance in MOF-based materials. Here, we choose AlFFIVE-1-Ni, a MOF with a one-dimensional channel, as the filler in the polymer matrix and use our previously developed computational methods to construct a series of MOF/Polymer interfaces with the selection of both rigid and more flexible polymers. Subsequently, we performed Grand Canonical Monte Carlo and our recently proposed concentration gradient-driven molecular dynamics (CGD-MD) simulations to assess the thermodynamic and dynamic adsorption properties of these MMMs. Our simulations revealed that the distinct characteristic of polymer backbones result in different interfacial void regions. We evidenced that not only the size but also the shape of the interfacial voids region have eminent effects on the gas transport properties of the MMMs with respect to a selected range of molecules, e.g. CO2, N2 and CH4. Our results constitute an important step toward the rational design of MMMs with the optimal interfacial void size/shape to achieve the highest performance for the separation of industrially relevant gas separations.

Recent Publications

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Biography

Guillaume Maurin, received his PhD in Physical Chemistry from Université Montpellier 2 (France) in 2001. After a Post-Doctoral Marie Curie Fellowship at the Royal Institution of Great Britain in London (U.K.) in the group of Pr. C.R.A. Catlow, he became Lecturer in 2002 at the Université Provence-Marseille (France) and later at the Université Montpellier 2 where he received his "Habilitation to Direct Research" in 2006. He is currently Professor at the Université Montpellier and at the Institut Universitaire de France. He is head of the Axis Adsorption/interfaces of the Department Porous & Hybrid Materials at the Institut Charles Gerhardt Montpellier and his research interests include the development and applications of advanced molecular simulations techniques to design new nanoporous materials and related membranes, and model their performances for energy and environment-related applications.

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