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Computational-aided development of MOF 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 the MOF/polymer interface and gas transport through the MMMs is of significant importance. Here, we selected a series of MOFs, as fillers and use our previously developed computational methods to construct MOF/Polymer interfaces with the selection of both rigid and more flexible polymers. Subsequently, we performed Grand Canonical Monte Carlo and 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. CO_2, N_2 and CH_4. 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 (maximum 5)

1. Rational design of mixed-matrix metal-organic framework membranes for molecular separations, S.J. Datta, A. Mayoral, N. Murthy Srivatsa Bettahalli, P.M. Bhatt, M. Karunakaran, I. D. Carja, D. Fan, P. Graziane M. Mileo, R. Semino, G. Maurin, O. Terasaki, M. Eddaoudi, Science, 2022, 376, 6597, 1080.
2. Engineering MOF surface defects in mixed matrix membranes: An effective strategy to enhance MOF/polymer adhesion and control interfacial gas transport, D Fan, A Ozcan, O Shekhah, R Semino, M Eddaoudi, G Maurin, **Journal of Membrane Science Letters** 2022, 2 (2), 100029
3. Asymmetric pore windows in MOF membranes for natural gas valorization, Sheng Zhou, Osama Shekhah, Adrian Ramírez, Pengbo Lyu, Edy Abou-Hamad, Jiangtao Jia, Jiantang Li, Prashant M Bhatt, Zhiyuan Huang, Hao Jiang, Tian Jin, Guillaume Maurin, Jorge Gascon, Mohamed Eddaoudi**, Nature** 2022, 606, 7915, 706.

Biography

Guillaume Maurin, received his PhD in Physical Chemistry from Universite Montpellier 2 (France) in 2001. After a Post-Doctoral Marie Curie Fellowship at the Royal Institution of Great Britain in London (UK) in the group of Pr. C. R. A. Catlow, he became Lecturer in 2002 at the Université Provence-Marseille (France). He is currently Full Professor at the Université Montpellier and member of the Institut Universitaire de France. His research interests include the development and applications of advanced molecular simulation techniques to design advanced nanoporous materials and related membranes for energy and environmental applications.

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