Prediction of physical properties for the design of processes in the oil & gas industry using molecular simulation

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Accurate knowledge of the physical properties of complex chemical systems is of extreme importance for the design and optimization of industrial processes. The unprecedented increase of computing power in the last couple of decades, the development of efficient algorithms and methods, and advances in molecular force fields have made molecular simulation a powerful tool in predicting such properties very accurately, and often with very limited experimental information involved. Related to this, molecular simulation can be used for the design of new materials with improved, often tailor-made, properties compared to existing materials. In this lecture, a few representative examples from recent work related to the oil & gas industry will be discussed.

Gas separation is considered as one of the most important industrial processes: 45 - 55% of the global energy consumption by the chemical industry, and 40 - 70% of the total capital and operating cost of the industry refer to separations. Zeolitic-imidazolate frameworks (ZIFs) have gained impressive popularity for gas separation in recent years. We have employed a combination of computational methods including Molecular Dynamics and Monte Carlo simulations, and Transition State Theory calculations for the prediction of gas separation efficiency of various ZIFs. Diffusion and solubility of various gases in ZIFs control such efficiency and are calculated here.

These simulation methods combined with accurate ab initio calculations for the development of new molecular force fields are used for the molecular design of new ZIFs for gas separations. We will show that a systematic metal substitution of Zn metal in ZIF-8 with other metals, including Co, Be, and Cd, results in orders of magnitude improvement in separation of mixtures such as n-alkane/iso-alkane, CO_2/ethane, CO_2/methane and CO_2/N_2 [1]. Another strategy refers to the replacement of the linker in the ZIF with a different one that results in substantial change in the aperture size of the ZIF. Such change alters the selectivity of the ZIF towards a particular gas separation dramatically. An example refers to the partial replacement of the 2-methylimidazolate (mIm) linker in ZIF-8 with benzimidazolate (bIm) resulting in ZIF-7-8 (Fig. 1). ZIF-7-8 exhibits remarkably high diffusion selectivities for CO_2/N_2 and CO_2/CH_4. This approach can be extended to other ZIFs and for other gas separations of industrial importance. New structures are expected to guide experimental work in the future.

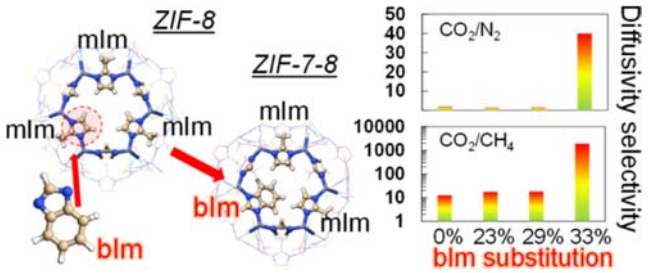

Figure 1. (left) Partial replacement of the 2-methylimidazolate (mIm) with benzimidazolate (bIm), (right) diffusivity selectivity for CO_2/N_2 and CO_2/CH_4 as a function of the bIm substitution.

References

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