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Diseño de Procesos de Adsorción para Separación de Gases utilizando Cristales Porosos

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Gas separation is essential for energy production. In the petroleum industry, isomerization processes generate a mixture of isomers of alkanes that require separation and recycling. There are other possibilities of obtaining refined fuels from raw material different from petroleum that also require gas separation. For example, the Fischer Tropsch Gas To Liquid (FT GTL) process provides liquid hydrocarbons from coal, biomass or natural gas. The process can be optimized by recycling compounds of the flue gas mixture. Related to energy and carbon capture and storage, the separation of hydrogen from carbon dioxide or the effective separation of carbon dioxide, carbon monoxide and oxygen are also essential. Ordered crystalline porous materials, such as zeolites, metal organic frameworks (MOFs) or zeolitic imidazolate framework (ZIFs) offer the potential for selective adsorption exploiting differences in molecular configurations. Zeolites are readily available, very stable and cheap. MOFs and ZIFs are less stable than zeolites, but they exhibit almost unlimited structural possibilities because of the wide variety of combinations of metal atoms, organic linker molecules and the building blocks used in self-assembly during synthesis.

We design conceptual separation processes consisting of several adsorptive steps using a combination of experiments and simulations. Molecular simulation is currently fast and accurate enough to allow rapid evaluation of structures for storage and/or separation devices. For effective separation, one needs to find materials with high adsorption selectivity and with the adequate capacity for use in traditionally used fixed-bed devices. Hence, crystalline structures need to be examined for their ability to conduct

gas separation based on adsorption equilibrium, selectivity, diffusion, permselectivity, structural features and kinetics. In most cases the efficiency mostly depends on the optimal combination of selectivity and effective pore volume, and this can be obtained from our simulations and experiments. Using this approach, we designed for example, a double-layered ZIF membranes fabricated inside polyimide P84 hollow fibers for the separation of hydrogen/carbon dioxide mixture (Figure 1). Our hypothesis is that a carbon dioxide adsorption reduction on the surface of the ZIF-9 would enhance the molecular sieving effect of this ZIF layer and therefore the selectivity in the hydrogen/carbon dioxide mixture separation of the entire membrane [1]. Similarly, we found zeolites and MOFs that could be effective materials for the separation of hydrocarbons (e.g. alkanes from alkenes and structural and chiral isomers), and we targeted some zeolites that combined in the correct order could optimize the syngas process, purify natural gas or enhance the capture of carbon dioxide and the recovery of carbon monoxide from gas mixtures [2-4].

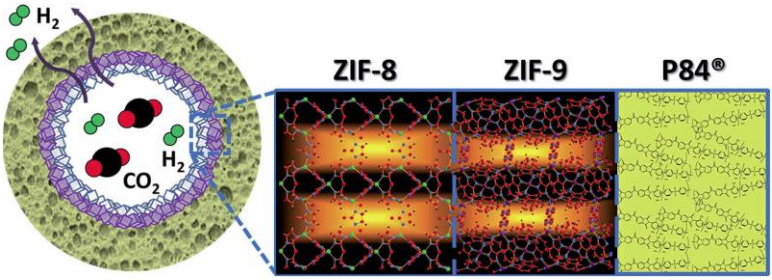

Figure 1. Scheme of the double-layered ZIF-8/ZIF-9 membrane inside a polymeric (P84) hollow fiber for H_2/CO_2 separation

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