Advancing Precision Molecular Sieving in Metal-Organic Framework Membranes through Targeted Material Manipulation

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From producing clean CH_4 and H_2, raw materials for high-quality plastics, manufacturing of semiconductors, CO_2 capture or fundamental research on Helium-hungry devices, gas separation is of crucial importance for our modern society. To isolate specific gases from their mixtures and increase their purity, energy-intensive cryogenic distillation techniques are widely applied. Instead of relying on cryogenic distillation, membranes can serve as an alternative, functioning only as physical barriers within a gas stream with up to 80% increased energy efficiency. These membranes operate based on the chemical potential gradient, with their potential being unlocked by the materials' properties.

Metal-organic frameworks (MOFs), a class of reticular hybrid materials consisting of metal nodes or clusters bridged by organic linker molecules, are highly tailorable porous materials. Among the up to now >100,000 MOF structures, a good fraction offers the desired chemical and thermal stability for membrane processes, but reticular chemistry is often not enough to provide precise molecular sieving features.

To separate the smallest gases, from H_2, He, CO_2, N_2, CH_4, and C_2, to C_3 hydrocarbons based on their kinetic diameter, we are on the hunt for high-precision molecular sieves and find ways to manipulate the porosity of MOFs on the sub-Ångström range. We use light-induced switches and electric fields to manipulate the pore gate, eliminate soft porosity or utilize breathing in these frameworks. Melting MOFs into nanoporous glasses through thermal processing enables us to make large monolithic films with precise molecular sieving cut-off.

Zooming out of the pore, we also focus on various methods of materials manipulation to translate the desired features into cm-scale membranes through liquid processing. For example, by using N-heterocyclic carbenes MOF nanoparticles can be ligand exchanged. This leads colloidal solutions with permanent porosity, or so-called “porous liquids,” which can be applied for gas separation by themselves. Furthermore, colloidal dispersions enable us to cast high-quality polymer-filler mixed matrix membranes.

The last step is to find ways to mature the technology developed in our lab and test our prototypical membranes for the different gas separation applications. For this purpose, lithographic 3D printing is applied, which we use to print synthesis equipment, measurement devices and the membrane substrates themselves.