

High-Throughput Screening of Metal Organic Frameworks (MOFs) for CO₂ separation

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The CO₂ capture from fossil fuel combustion flue gas is the focus of significant research efforts. The existing technologies are extremely energy intensive, including amine absorption and pressure-swing adsorption. Metal-organic frameworks (MOF) are strong candidates as size-selective, high-capacity materials for separation of CO₂ and other gases. MOFs exhibit nanoporous crystalline structure in which organic linker molecules self-assemble with metal cations to form extended crystals with well-defined pore size, high surface area, low framework density, and thermal stability. These properties make MOFs an attractive alternative to traditional zeolite materials for gas separation in membrane separation technologies.

In principle, a potentially infinite number of MOFs with various combinations of organic linker and metal cation present opportunity to tailor pore structure, size, and functionality for CO₂ capture from flue gas. Most previous work reports only single gas adsorption with a small number of samples, which limits the fast selection of promising candidates among the huge number of the available MOFs. Even when water stability is reported, it is usually based on structure, not adsorption selectivity. Similar problems confound determination of other contaminant effects, e.g., acid gases like SO₂ and NO₂. To address these challenges, a novel parallel high-throughput (HT) sorption screening system is presented, which enables efficient screening of MOFs based on CO₂/N₂ adsorption and diffusion selectivity, as well as their sensitivity to water vapor and acid-gases.