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UUltra-Microporous MOFs for Selective CO_2 Capture from Industrial Gas Mixtures

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Though several potential applications of Metal Organic Frameworks (MOFs) have been demonstrated, still gas separation and storage remains the most developed and highly promising one. MOFs with ultra-micropores are typically made of small rigid ligands and hence exhibit significant rigidity, inherent molecular sieving and exceptional chemical and thermal stabilities. Their ability to form as high quality single crystals enables their atomic level structural characterization via crystallography and this makes them amenable for structural and chemical tuning via pre-designed chemistry. We have recently via a 'by design' approach made ultra-microporous MOFs with remarkably high CO2 capacity and selectivity under conditions relevant to pre- and post-combustion CO2 capture. This makes them highly promising candidates for removal of this greenhouse gas from large scale sources via the well-established pressure/vacuum swing technology. We have investigated the low/high pressure CO2 capture capabilities of the MOFs under static and dynamic conditions. The crystal structure of the MOFs facilitate the use of extensive simulation based modeling. In fact, we have developed a combined experimental-simulation approach in which using single crystal X-ray diffraction we locate the specific adsorption site within the MOF and utilizing this as a model we have developed simulation routines that enable the identification of adsorption sites in a variety of other MOFs that show high affinity for a specific gas. With this optimized approach, we have developed superior MOFs and identified the site-specific interactions of CO2 within the confinements of such MOFs using atomic-simulations. Furthermore, we simulated the crystal structure of a variety of MOF with low energy conformations and a detailed calculation of the 'parasitic energy' associated with the CO2 capture process using different MOFs, including our MOF, as sorbent suggests our MOF as a molecular sponge with record-low parasitic energy. Parasitic Energy is a wholesome metric that defines the parasitic load the capture process would impose on a power plant.

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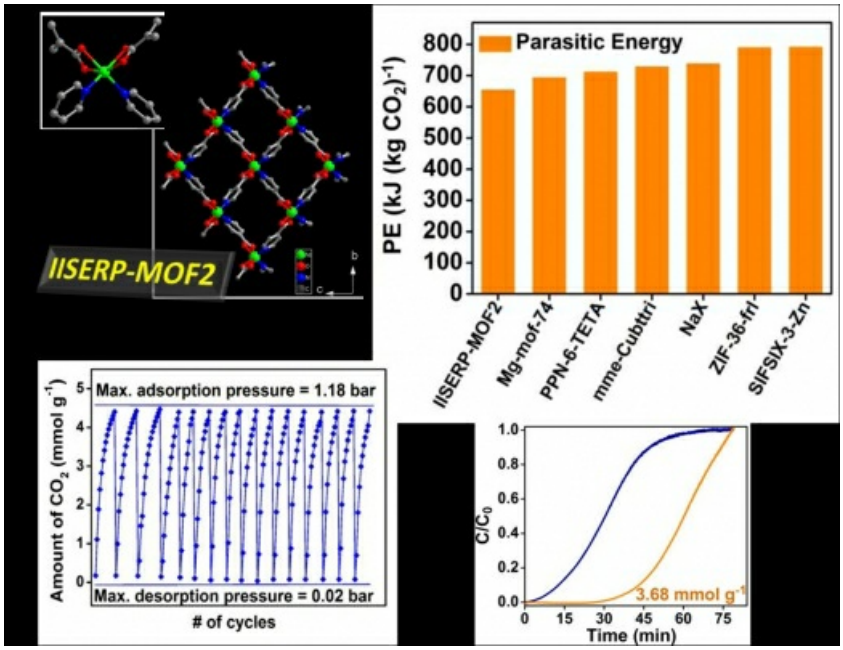

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