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Comparative study of metal-organic frameworks for carbon capture applications JASON SIMMONS, WEI ZHOU, HUI WU, TANER YILDIRIM, NIST Center for Neutron Research — With the current prevalence of hydrocarbon-based energy sources, carbon capture and sequestration are essential technologies for minimizing the emission of carbon dioxide and the resulting increased atmospheric concentration of CO₂. Current technologies based on absorption require high temperature regeneration of the solvent, ultimately leading to significantly decreased efficiency and increased cost. Development of an adsorption-based technology, based on physical adsorption in optimized porous media, would greatly reduce the regeneration costs. Here we discuss the carbon capture performance of a range of metal-organic frameworks (MOFs), including both high surface area materials as well as those with sites that have been engineered to have enhanced binding. In particular, we demonstrate that MOFs can capture significant amounts of CO₂ and that the CO₂ can be readily removed from the MOF using standard pressure/vacuum swing techniques, yielding cyclic capture capacities in excess of 5 mmol/g. Further, we discuss the role of pore geometry and surface chemistry in the capacity of CO₂ that can be removed in order to best optimize these materials. Lastly, we will address the effect of flue gas impurities on the carbon capture performance of these MOFs.

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