Neutron and X-ray Scattering to Characterize Adsorbents and Their Hosts

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Adsorption of molecules in functionalized and high surface area metal-organic frameworks (MOFs) is of emergent technological importance in a multitude of areas ranging from chemical separations to energy storage. We have been studying the properties of MOFs and other porous materials for storage and separations of industrially important small molecules such as hydrogen, oxygen, carbon dioxide, noble gases, and short chain organics. Besides the geometrical and porosity control available in MOF chemistry, the properties of the frameworks can be tweaked to elevate electrostatic interactions by exposing open metal cation sites or through enhanced van der Waals contacts via functionalizing ligands and introducing flexibility. We will highlight some of the most recent results on optimized interactions of hydrogen with open metal sites to obtain room temperature adsorption and a range of dynamic frameworks pore binding in MOF-like materials that optimize hydrogen adsorption using close-contacts, small pore MOFs which are robust to moisture and are highly selective for a series of separations, and MOF-like materials with flexible response of the pore geometries on adsorption. These results illustrate the governing characteristics of these material properties and the interactions with the guest molecules.