

Neutron Diffraction: A Unique Technique to Study Gas Adsorption in Functional Porous Crystalline Materials

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Porous metal-organic frameworks (MOFs) are promising material candidates for gas separation. Recently, some flexible MOFs were found to exhibit interesting gas separation properties. Rational design of new flexible framework materials targeting for this application requires fundamental mechanistic understanding of the gas-framework interaction and the nature of the framework flexibility. X-ray single crystal diffraction and powder diffraction are widely used to characterize these materials and study their gas adsorption structures. Neutron diffraction is a technique often complementary to x-ray diffraction. In some cases, neutron diffraction can provide unique information not available from x-ray. In this talk, I am going to first briefly compare neutron diffraction with x-ray diffraction. I will present our recent work using neutron diffraction to understand the gas adsorption in several newly developed flexible porous framework materials, where neutron diffraction was found to play a unique and powerful role. The insights obtained from our studies provide important guidance for the development of new flexible framework materials aiming for improved gas separation properties.