

Structural Resolution of H₂ and D₂ Within Metal-Organic Frameworks Using Neutron Diffraction

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Metal-organic frameworks are a class of adsorbents which can potentially engender H₂ storage above cryogenic temperatures. These materials can leverage undercoordinated metal sites to produce strong associations with H₂ molecules, or they can be leverage small pores framework associations to trap H₂ gas. Regardless of gas adsorption, structural determinations of metal-organic frameworks through powder diffraction, whether X-ray or neutron, are generally complicated given each material's often-large unit cell and complex organic moieties. Introduction of gas molecules into the porous materials undoubtedly furthers refinement complication. To facilitate success, careful experimental conditions as well as careful refinement parameters must be considered. In this talk, I will discuss neutron diffraction work done by our team on leading metal-organic framework materials for hydrogen storage, and how to best deal with often delicate refinements.