PHYSICAL ASPECTS OF HYDROGEN ADSORPTION  
IN MICROPOROUS MATERIALS

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Abstract  
Physico-chemical adsorption of molecules in microporous materials has long been used in industrial processes and significant efforts have been expended in understanding the myriad of structure-property relationships of interest. Efforts are currently being applied to understand the adsorption behavior in potentially industrially and environmentally important systems such as zeolitic and metal-organic type frameworks. For instance, hydrogen storage materials must achieve higher gravimetric and volumetric densities than those currently available in order to achieve a viable storage system that can be reversibly refueled. Although the storage capacities of metal-organic frameworks (MOFs) have progressed significantly over recent years, some technological obstacles pose challenges for their future improvement. Similar claims are also true regarding carbon dioxide capture and sequestration, with difficult questions being raised about how to deal with the end products.

We will show how neutron powder diffraction methods coupled with spectroscopic tools, are invaluable to advancing our understanding the performance (or lack of performance) of candidate storage materials and systems. This will be illustrated by discussing several examples taken from our recent research involving MOFs, nano-structured carbon-based materials and zeolites.

Figure 1. Ball and stick model showing D\textsubscript{2} adsorption sites (labeled I-III) in a Fe containing MOF, Fe\textsubscript{2}(dobdc).