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Enhancing the interaction strength and capacities of hydrogen storage via surface adsorption CRAIG BROWN, NIST Center for Neutron Research

Storing Hydrogen molecules in porous media based on a physisorption mechanism is one possible approach to reach the US Department of Energy targets for on-board hydrogen storage. Although the storage capacities of metal-organic frameworks (MOFs) have progressed significantly over recent years, some technological obstacles pose challenges for their future improvement. These include the generally low H₂ adsorption enthalpy limiting room temperature applications and the lack of understanding of surface packing density hindering the efficient improvement of H₂ adsorption uptake. To improve the H₂ affinity in MOFs, our previous work has shown that the coordinatively unsaturated metal centers (CUMCs) can greatly enhance the H₂ binding strength. Our current study of MOF-74 will be presented, showing that its open Zn^{2+} ions bind H₂ strongly and are identified as being responsible for the large initial H₂ adsorption enthalpy of 8.4 kJ/mol. In all, there are four H₂ adsorption sites in MOF-74 identified by neutron powder diffraction. These four hydrogen adsorption sites are closely packed in MOF-74 and form a one dimensional nanoscale tube structure. We also demonstrate an interesting correlation that MOFs with CUMCs generally show larger surface packing densities than that of other MOFs without CUMCs. The implications of this will be addressed.