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Hydrogen molecule binding to unsaturated metal sites in metal-organic frameworks studied by neutron powder diffraction and inelastic neutron scattering[1] YUN LIU, NIST Center for Neutron Research; Dept. of Material Science and Engr., Univ. of Maryland, College Park, CRAIG BROWN, NIST Center for Neutron Research; Indiana Univ. Cyclotron Facility, DAN NEUMANN, NIST Center for Neutron Research, MIRCEA DINCA, JEFFREY LONG, Dept.of Chemistry, Univ. of California, Berkeley, VANESSA PETERSON, CAMERON KEPERT, School of Chemistry, The Univ. of Sydney — Metal organic framework (MOF) materials have shown considerable potential for hydrogen storage arising from very large surface areas. However, the low binding energy of hydrogen molecules limits its storage capability to very low temperatures (< 77 K), which is impractical for industrial applications. Using neutron powder diffraction (NPD), we have characterized the hydrogen adsorption sites in a selected series of MOF materials with exposed unsaturated metal ions. Direct binding between the unsaturated metal ions and hydrogen molecules is observed and responsible for the enhanced initial hydrogen adsorption enthalpy. The different metals centers in these MOFs show different binding strength and interaction distances between the hydrogen molecule and metal ions. The organic linker also affects the overall H_2 binding strength. Inelastic neutron scattering spectra of H_2 in these MOFs are also discussed.

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