

Probing Structure, Bonding, and Dynamics in Hydrogen-Storage Materials by Neutron-Scattering Techniques

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The novel properties of the neutron, such as its large scattering cross section for hydrogen, can be routinely exploited by a variety of experimental neutron methods in order to probe the amount, location, bonding states, and motion of hydrogen in any promising hydrogen-storage material. For example, neutron powder diffraction (NPD) is critical for probing the structural details of hydrogen-storage materials and locating the positions of the absorbed hydrogen atoms and/or molecules. Neutron vibrational spectroscopy (NVS) complements NPD structural studies by revealing the local bonding potentials of the absorbed hydrogen. Quasielastic neutron scattering (QENS) provides molecular-scale spatial and temporal (10^{-8} - 10^{-14} s) information simultaneously on diffusive motions of hydrogen in hydrogen-storage materials, and as such, provides valuable insights about the molecular-scale geometry and timescale of the diffusion mechanism. The results of various neutron-scattering measurements can, in turn, be used to validate the fundamental physical description resulting from first-principles computational methods and thus deepen our overall understanding of the technologically important materials properties. This talk will provide recent examples of combined neutron and computational studies of new hydrogen-storage materials performed at the NIST Center for Neutron Research, including destabilized light-metal hydrides and metal-organic-framework structures.