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Probing Structure and Bonding in Hydrogen-Storage Materials by Combined Neutron-Scattering Techniques and First-Principles Calculations. T.J. Udovic, NIST Center for Neutron Research, National Institute of Standards and Technology, 100 Bureau Dr., MS 8562, Gaithersburg, MD 20899-8562 USA.

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. The results of both NPD and NVS measurements can 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 alkaline and alkaline-earth hydrides and metal-organic-framework structures.