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A Study of the Structural and Dynamical Properties of Lithium Borohydride Confined within Nanoporous Framework Structures using Neutron Scattering Investigations CERIS HAMILTON, MICHAEL R. HART-MAN, University of Michigan, HUI WU, University of Maryland / National Institute of Standards and Technology, TERRENCE J. UDOVIC, National Institute of Standards and Technology, JOHN. J. RUSH, University of Maryland / National Institute of Standards and Technology, ADAM F. GROSS, HRL Laboratories LLC, JOHN J. VAJO, HRL Laboratries LLC, THEODORE F. BAUMANN, Lawrence Livermore National Laboratory — Lithium borohydride, LiBH₄, is a complex metal hydride that shows great promise as a hydrogen storage medium with a volumetric hydrogen density of 122 kg H/m^3 and a gravimetric hydrogen density of 18.5 wt. %. We have previously reported on the structural and dynamical properties of neat ⁷Li¹¹BH₄ as determined by neutron powder diffraction, neutron vibrational spectroscopy, and quasielastic neutron scattering. Here we report on recent measurements undertaken to investigate the changes in the structural and dynamical properties that are observed when this material is confined within nanoporous structures with pore sizes ranging from 4 nm to 25 nm. These materials exhibit a reduction in the structural transition and melting temperatures, which we associate with a marked decrease in the activation energy for reorientational motions of the $[BH_4]^-$ tetrahedra.

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