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Structure and librational dynamics in borohydrides MONIKA HARTL, Los Alamos National Laboratory, MICHAEL WOLVERTON, University of Arkensas - Little Rock, ALICE ACATRINEI, Los Alamos National Laboratory, ABHIJIT BHATTACHARYYA, University of Arkansas - Little Rock, LUKE DAEMEN, Los Alamos National Laboratory — Borohydrides are candidates for reversible hydrogen storage. The attention accorded to this class of materials is supported by extensive hydrogenation/dehydrogenation thermodynamic measurements. However, the underlying chemical reaction mechanisms remain uncertain. We used neutron diffraction and inelastic neutron scattering, together with a computational approach, to examine the connection between structure and dynamics in several borohydrides and the possible role played by dynamics in the approach to the dehydrogenation transition state.

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