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Dehydrogenation of $NaAlH_4$ from First-principles Molecular Dynamics BRANDON WOOD, NICOLA MARZARI, Department of Materials Science and Engineering, MIT — Key among the materials challenges facing a hydrogen economy is the discovery of lightweight materials for reversible hydrogen storage in the solid state. Although chemical and metal hydrides have been under intense investigation, progress has been curtailed by a lack of understanding of the reaction paths for hydrogenation and dehydrogenation in such materials. We present here our first-principles molecular dynamics results for $NaAlH_4$, one of the promising and most extensively studied candidates for hydrogen storage. We analyze proton transport in the presence of a variety of low-energy defects and surfaces, and we discuss possible candidates for the key mechanisms of dehydrogenation in the material. The results are presented in terms of the structural phase transition to α-Na_3AlH_6.

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