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Hydrogen Storage in Ti-doped NaAlH₄. E.H. Majzoub¹, K.F. McCarty¹, R. Stumpf¹, S. Spangler¹, K.J. Gross¹, G.D. Sandrock¹, J. Herberg², R. Maxwell², V. Ozolins³, ¹Sandia National Laboratories, Livermore, CA, ²Lawrence Livermore National Laboratories, Livermore, CA, ³Univ. of California, Los Angeles, CA.

The realization of a true hydrogen economy depends on many materials science breakthroughs, one of which is the storage of hydrogen at benign temperatures and pressures. While some interstitial metal hydrides excel in this regard, they are typically around 2 wt.% H₂. There is a class of complex (polar-covalent bonded) hydrogen storage materials based on AlH_x and BH_x anions with much larger hydrogen wt. % that is gaining wide attention. NaAlH₄ has been the focus of this attention due to the discovery that it can be made reversible by the addition of transition metal dopants (Bogdanovic, 1997). The kinetics of the decomposition and reformation are increased many orders of magnitude by the addition of around 1-4 at.% Ti. We present an overview of the hydrogen sorption properties of Ti-doped sodium alanate, and a detailed characterization of the lattice dynamics of the material using Raman spectroscopy, through a polarization analysis of single crystal NaAlH₄. In addition, high temperature, in-situ Raman measurements are shown to indicate a very stable AlH₄ anion in un-doped (pure) NaAlH₄.