

X-ray and Neutron Diffraction Studies of Ti-doped Sodium Aluminum Hydride, a Promising New Hydrogen Storage Material. Craig M. Jensen^a, Sesa S. Srinivasan^a, Martin Sulic^a, Hendrick Brinks^b, Bjorn Hauback^b, Job T. Rijssenbeek^c, Yan Gao^c, Klaus Yvon^d, Cerny Radovan^d, and Alberto Albinati^e. a)Dept. of Chemistry, Univ. of Hawaii, Honolulu, HI 96822 USA, b)Inst. for Energy Technology, Kjeller, NO-2027 Norway, c)GE Global Research, Niskayuna, NY 12309, d)Laboratoire de Crystallographie, Univ. de Geneve, Geneve 4, Switzerland, e)Dept. of Structural Chemistry, Univ. of Milan, I-20133 Milan, Italy.

In 1997, Bogdanovic reported that hydrogen could be reversibly evolved from solid NaAlH_4 under moderate conditions upon doping the hydride with a few mole percent of selected transition metal complexes. In order to elucidate the mechanism of the reversible, solid state decomposition of the doped hydride to NaH/Al , we have probed the doped and undoped hydride through synchrotron X-ray and neutron diffraction as well as: tunneling and scanning electron microscopy; density functional calculations; infrared, electron paramagnetic resonance, X-ray absorption and anelastic spectroscopy; and kinetic studies. A model of the doped hydride has evolved from these studies in which titanium dopants, proximal to the complex aluminum hydride anions, generate highly mobile point defects that lead to the enhanced hydrogen cycling kinetics. The details the synchrotron X-ray and neutron diffraction studies will be presented and discussed in terms of their relationship to the results we have obtained through the other techniques and the emerging mechanism of reversible elimination of hydrogen from the doped hydride.