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Structure and Bonding in Destabilized Metal Hydrides for Hydrogen Storage.

HUI WU, University of Maryland and NIST Center for Neutron Research

Light-metal hydrides possess high hydrogen-storage capacities (> 5 wt.%), but their utility is generally compromised by high thermal stability, rather slow absorption kinetics, and/or problems with reversibility for hydrogen absorption/desorption cycling. There has been great emphasis, particularly in recent years, on attempts to destabilize and otherwise improve the properties of these hydrides by alloying with Si and other elements. We describe here the study of lithium and calcium hydrides alloyed with Si and Ge using ball-milling techniques. The details of the structure and bonding of the Li/Si/H(D), Li/Ge/H(D) and Ca/Si/H(D) systems have been revealed through a combination of neutron and x-ray diffraction, neutron spectroscopy and first-principles calculations. We report the discovery of several new hydride phases, the nature of Si-H bonding in these hydride systems and the effects of amorphization in the Ca/Si/H alloys. The implications of our results for future investigations will be discussed.