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Hydrogen Bonding in CaSiH(D)$_{1+x}$: Is there Covalent Character? T. J. UDOVIC, H. WU, W. ZHOU, J. J. RUSH, T. YILDIRIM, NIST Center for Neutron Research — We report here our neutron powder diffraction and neutron vibrational spectroscopy study of CaSiH(D)$_{1+x}$ along with first-principles calculations, which reveal the hydrogen structural arrangements and bonding in this novel alloy hydride. Both structural and spectroscopic results show that, for x >0, H(D) atoms start occupying a Ca_3Si interstitial site. The corresponding Si-H(D) bond length is determined to be 1.82 Å, fully 0.24 Å larger than predicted by theory. Here we discuss in detail our neutron spectroscopic measurements, which are also generally at odds with strongly covalent Si-H bonding in CaSiH$_{1+x}$ that such calculations suggest. These results may have implications for a number of ongoing studies of metal-hydrogen systems destabilized by Si alloying.

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