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Identification of the Amorphous AlB_4H_{11} Structure[1] YONGLI WANG, YONGSHENG ZHANG, Northwestern University, XUENIAN CHEN, JICHENG ZHAO, The Ohio State University, WEI ZHOU, TERRENCE UDOVIC, National Institute of Standards and Technology, C. WOLVERTON, Northwestern University — In recent experimental work, AlB_4H_{11} has been identified as a potential hydrogen storage material with a good desorption temperature and partial reversibility. It is an amorphous, white solid at room temperature and its molecular structure is presently unknown. We combine experimental measurements (NMR, neutron vibrational spectra and IR) and a theoretical structure prediction method to identify the (local) structure of the amorphous AlB_4H_{11} phase. The theoretical structure prediction method is a combination of the Monte-Carlo based prototype electrostatic ground state search (PEGS) method and first-principles calculation (DFT). The PEGS+DFT method has successfully predicted many crystalline solid structures, but has never been applied to the prediction of amorphous solid structures. The PEGS predictions of the AlB_4H_{11} structure are quite successful: we find the calculated phonon density of states (pDOS) of our PEGS+DFT predicted structures is in close agreement with the experimental vibrational measurements. More broadly, our findings indicate that first-principles theoretical design of new amorphous materials for energy storage is now possible, paving a promising way for similar studies in the future.

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