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Prediction of a Stable Solid Boron Hydride for Onboard Hydrogen Storage[1] TESFAYE ABTEW, PEIHONG ZHANG, Department of Physics, University at Buffalo, State University of New York, Buffalo New York 14260, USA — We present a first principles study of a new solid boron hydride structure that contains more than 9 wt. percentage of hydrogen for its potential for hydrogen storage. The structural, electronic and dynamic properties are calculated using density functional theory based electronic structure methods. In addition to its high gravimetric capacity, the structure has several desired properties for onboard hydrogen storage: (1) The bonding between boron and hydrogen is relatively weak, which can be weakened further upon charge doping; (2) A stable backbone boron network is favorable for reversible hydrogenation and dehydrogenation. The proposed synthetic route of this solid boron hydride as well as the hydrogen release kinetics will also be discussed.

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