

Structure and Dynamics of Ammonia Borane

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Amine boranes are attractive candidates for the storage of high volumetric and gravimetric densities of hydrogen for fuel cell powered devices. The parent compound, ammonia borane (NH_3BH_3), isoelectronic with ethane, yet it is a solid molecular crystal under standard conditions. Ammonia borane is stable at room temperature but will desorb >15 mass% hydrogen at moderate temperatures. Our group has been investigating the thermal and catalytic mechanisms of amine borane decomposition leading to hydrogen formation. We believe that the interactions between the hydridic BH and protic NH hydrogen are responsible for the low activation barriers for hydrogen desorption. In this presentation we will discuss our experimental and computational research aimed at developing a fundamental understanding of the chemical and physical properties of these hydrogen rich materials. This work is supported by the US Department of Energy, Basic Energy Sciences Hydrogen Fuel Initiative. Battelle operates PNNL for DOE.