

Abstract Submitted  
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**First-Principles Prediction of Hydrogen Storage Energetics in the Li-B-N-H System**<sup>1</sup> WENHAO SUN, CHRISTOPHER WOLVERTON, Northwestern University, VIDVUDS OZOLINS, University of California, Los Angeles — In this talk, we describe recent efforts using first-principles density functional theory (DFT) based methods to elucidate the reaction energetics and phase stability in the Li-B-N-H hydrogen storage system. We have calculated DFT total energies of a large number of phases in this system, including  $\text{Li}_4\text{BN}_3\text{H}_{10}$ ,  $\text{Li}_2\text{BNH}_6$ , and their decomposition products. We then use these DFT energies in the recently developed “grand canonical linear programming” (GCLP) approach to automatically detect the thermodynamically preferred decomposition paths of these compounds as functions of temperature and  $\text{H}_2$  pressure. Using the combined DFT+GCLP approach we calculate thermodynamic phase diagrams in the  $\text{LiBH}_4 - \text{LiNH}_2$  phase space. Some phases (e.g.,  $\text{Li}_3\text{BN}_2$ , BN) are found to be very energetically stable, but are often only seen experimentally at very high temperatures, presumably due to hindered kinetics. By removing these phases from the DFT+GCLP calculations and examining the resultant phase diagrams, we can provide insight into the experimental reaction mechanisms.

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