

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**First-principles investigations of the quaternary Li-Zn-B-H hydrogen storage system** YONGLI WANG, CHRIS WOLVERTON, Northwestern University — Mixed metal borohydride hydrogen storage materials are a new class of materials which may possess better thermodynamic and kinetic properties than their separate phases.  $LiBH_4$  has an undesirably high  $H_2$  desorption temperature, while  $Zn(BH_4)_2$  has a lower desorption temperature, but releases  $B_2H_6$  upon desorption. We have used density functional theory, as well as Monte Carlo-based crystal structure prediction tools and phase diagram computational methods to explore the stability and decomposition reactions of mixed Li and Zn borohydrides to ascertain whether they possess an intermediate decomposition temperature. Based on a combination of classical potentials, Monte Carlo optimization, and DFT calculations, we search for low-energy quaternary borohydrides as a function of the Li/Zn context. We find that this system has compounds that are lower in energy than the isolated borohydrides. In agreement with prior work, we confirm the existence of a  $LiZn(BH_4)_3$  compound, which as yet has been unobserved. We find that this new mixed compound  $LiZn(BH_4)_3$  decomposes via an initial decomposition of  $Zn(BH_4)_2$ , and a subsequent decomposition of  $LiBH_4$ . This sequential decomposition is favored due to the lack of stable intermediate products which involve both Li and Zn. Using this framework, we are searching for stable mixed metal borohydrides in a wide variety of other systems.

Yongli Wang  
Northwestern University

Date submitted: 19 Nov 2010

Electronic form version 1.4