Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Hydrogen release reactions in the {H,Li,B,Na,Al} system ERIC DHALL, Graduate Student, VIDVUDS OZOLINS, Professor — A thermodynamic investigation of the {H,Li,B,Na,Al} system for new solid state hydrogen storage reactions is performed using first-principles DFT calculations and the the grand-canonical linear programming approach (Akbarzadeh, et al. Adv. Mater. 2007, 19, 3233). We report the static, zero-point, and T > 0 K vibrational energies of all known compounds in this system. Enthalpies, entropies, and hydrogen release temperatures are calculated for all thermodynamically reversible dehydrogenation reactions occurring from 0-1000K. Several novel mixtures of reactants with high gravimetric hydrogen storage densities are found using the calculated {H,Li,B,Na,Al} phase diagrams.

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Date submitted: 16 Nov 2010 Electronic form version 1.4