Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

First-Principles Study of the Li-Na-Ca-N-H System: Compound Structures and Hydrogen-Storage Properties PATTANASAK TEERATCHANAN, FEI ZHOU, University of California, Los Angeles, KYLE MICHEL, Northwestern University, VIDVUDS OZOLINS, University of California, Los Angeles — Mixed-metal amides and imides are being widely investigated as potential hydrogen storage materials. Using a combination of first-principle DFT calculations, grand-canonical linear programming, and prototype electrostatic ground state (PEGS) approaches, we predict hydrogen storage reactions in the Li-Na-Ca-N-H system. The enthalpies, entropies, static, zero-point, and T>0K vibrational energies of known compounds together with our predictions of some incomplete experimental crystal structures are presented.

Pattanasak Teeratchanan
University of California, Los Angeles

Date submitted: 11 Nov 2011 Electronic form version 1.4