Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Ab initio investigation of $LiNH_2$, Li_2NH, and $Mg(AlH_4)_2$ complex hydrides BLANKA MAGYARI-KOPE, VIDVUDS OZOLINS, University of California, Los Angeles, Department of Materials Science and Engineering — First-principles calculations on the complex hydrides $LiNH_2$, Li_2NH, and $Mg(AlH_4)_2$ were performed to determine their structural stability, electronic structure and formation energy. All these compounds were recently reported the most promising materials for reversible hydrogen storage. We discuss the ionic character and binding implications of other complex hydrides. Possibilities to improve the hydriding/dehydriding reactions are presented.

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Date submitted: 30 Nov 2004 Electronic form version 1.4