Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

**Thermodynamic properties of LiAlH4 from first-principle calculations** XUEZHI KE, CHANGFENG CHEN, Department of Physics, University of Nevada, Las Vegas, NV 89154-4002, USA — The potential hydrogen-storage materials of LiAlH4, and Li3AlH6 have been studied by using density functional theory (at GGA level), and harmonic phonon approximation. The thermodynamic properties of these materials have been studied in detail. We found that the decomposition of LiAlH4 is not reversible, which may indicate that the direct synthesis of LiAlH4 may be not possible. The calculations indicate that Li3AlH6 can be used as a hydrogen-storage material under certain conditions. In addition, the phase diagram of these materials will be presented.

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Date submitted: 10 Nov 2006 Electronic form version 1.4