Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Lattice Dynamics and Thermodynamic Properties of Complex Hydride $NaAlH_4$ AMRA PELES, Georgia Institute of Technology, M. Y. CHOU, Georgia Institute of Technology — We present a first-principles investigation of the lattice dynamics and thermodynamical properties of the complex hydride $NaAlH_4$, a promising candidate for hydrogen storage. The calculations are performed within the density functional framework and using a linear response theory. Calculations of the phonon spectrum, Born effective charges Z* of the atoms, dielectric constants in high and low frequency limit are reported. The mode characteristics of zone-center phonons including LO-TO splitting are identified and compared to experiment. The quasiharmonic approach is used to study thermal expansion together with the mean square displacement of each atom and its relation to the melting point. The inclusion of the zero-point motion yields an expanded lattice compared to the static case, while the low-frequency correlated oscillations of Na and AlH_4 complexes are found to play an important role in destabilizing the lattice.

Mei-Yin Chou
Georgia Institute of Technology

Date submitted: 28 Nov 2004 Electronic form version 1.4