Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Structural Discrimination via DFT: Monoclinic Mg_2NiH_4 JAN HERBST, LOUIS HECTOR, JR., GM R&D Center — Mg_2NiH_4 is a semiconductor and forms an ordered low temperature monoclinic phase and a disordered high temperature cubic modification. Two distinct structures for the monoclinic phase from neutron diffraction studies of the deuterated analog, which we designate as LTI and LTII, are available in the published literature. We calculate the enthalpy of formation ΔH with density functional theory (DFT) for both using three different approximations for the exchange-correlation energy functional. Phonon spectra are calculated as well. DFT unequivocally identifies LTII as preferable since ΔH obtained for it is in better agreement with experiment and its phonon spectrum contains no anomalies. Structures approximating LTII derived from analyses of soft modes in LTI and in Mg-substituted $CaMgNiH_4$ are also discussed.

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Date submitted: 13 Nov 2008 Electronic form version 1.4