Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Ab initio electronic and lattice dynamical properties of cerium dihydride TANJU GUREL, RESUL ERYIGIT, Abant Izzet Baysal University — The rare-earth metal hydrides are interesting systems because of the dramatic structural and electronic changes due to the hydrogen absorption and desorption. Among them, cerium dihydride (CeH_2) is one of the less studied rare-earth metal-hydride. To have a better understanding, we have performed an ab initio study of electronic and lattice dynamical properties of CeH_2 by using pseudopotential density functional theory within local density approximation (LDA) and a plane-wave basis. Electronic band structure of CeH_2 have been obtained within LDA and as well as GW approximation. Lattice dynamical properties are calculated using density functional perturbation theory. The phonon spectrum is found to contain a set of high-frequency ($\sim$ 850-1000 cm^{-1}) optical bands, mostly hydrogen related, and low frequency cerium related acoustic modes climbing to 160 cm^{-1} at the zone boundary.

Tanju Gurel
Abant Izzet Baysal University

Date submitted: 20 Nov 2006 Electronic form version 1.4