Ab initio electronic and lattice dynamical properties of cerium dihydride

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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.

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Date submitted: 20 Nov 2006
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