p2

ELECTRONIC STRUCTURE OF SOME RARE EARTH DIHYDRIDES ß-RH_2 (R = La, Gd, Er)

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RÉSUMÉ

With the wien2k simulation code, we have performed *ab initio* calculations of electronic properties for some rare earth cubic stoichiometric dihydrides (ErH_2, GdH_2, LaH_2) using the full-potential linearized augmented plane wave method (FP-LAPW) approach within the density functional theory (DFT) in the generalized gradient approximation (GGA). Lattice parameters, bulk moduli, density of states and energy band structures in these compounds have been determined. In these dihydrides, the first two bands are separated by a gap of 0.7075 eV for ErH_2, 0.8708eV for GdH_2 and 1.0613 eV for LaH_2, from the metal *d* bands.

MOTS-CLÉS : rare earth, hydrides, dihydrides, wien2k, materials ab initio simulation, electronic structure calculations