Structural, elastic, electronic and chemical bonding properties of hydrides X2RuH6 (X = Mg and Ca): An ab initio study

O. Boudrifa, A. Bouhemadou

Abstract : Several applications of hydrides have been found so far, e.g. switchable mirrors [1–2], energy storage [3,4], rechargeable batteries [4], etc. Using first-principals density functional calculations, we have studied the structural, electronic elastic and elastic properties of the complex hydrides Mg2RuH6, Ca2RuH6. The calculated structural properties; namely equilibrium lattice constants, internal free parameters, bulk modulus and its first-order pressure derivative, are in good agreement with the available results. The relative changes of the structural parameters versus hydrostatic pressure have been investigated. The elastic constants and their pressure dependence are predicted using the static finite strain technique and the polycrystalline isotropic elastic moduli, namely bulk modulus, shear modulus, Young's modulus and Poisson's coefficient, Lames coefficients, average sound velocity and Debye temperature are numerically estimated in the frame-work of the Voigt–Reuss–Hill approximations. The mechanical stability of the considered materials has been examined on the light of the pressure dependence of the elastic constants. The elastic anisotropy of the X2RuH6 has been studied using three different methods. The analysis of the site and momentum projected densities, charge transfer and charge densities show that bonding is of covalent-ionic nature. The band structures show that all studied materials are indirect energy band gap semiconductors.

Keywords : structural, elastic, electronic, chemical bonding ab initio calculations, Electronic band, densities of states, Charge density.