ABSTRACT

Structural, mechanical, electrical and magnetic properties of novel do half-Heusler alloys CsXB (X = Sr, Mg and Z=B) are proposed by means of first-principles calculation based on the density functional theory (DFT). The exchange correlation functional is treated by the generalized gradient approximation proposed by Perdew–Burke–Ernzerhof (GGA-PBE). CsMgB and CsSrB are stable by SP. Our calculations show that CsMgB and CsSrB have a conducting nature incontrast, they show metallic behavior. Minority spin of CsMgB with band gap of 0.44 eV, whereas majority spin gap of CsSrB 0.34 eV. We found that these two compounds are mechanically stable. While CsSrB is brittle, CsMgB exhibits a ductile character. According to Slater-rule Pauling's (Mtot = (8 - Ztot) B). CsSrB has Mtot =2.00004μB and CsMgB with 2.00002. Nature of half-metals is obtained due to 2p states of Boron atom's spin polarization, whose p bands are primarily where the magnetic moment is generated. These compounds are good candidates in spintronics devices to study the properties of half-metallic ferromagnets due to the absence of transition metals.