

Disorder dependent half-metallicity in Mn₂CoSi inverse Heusler alloy

Abstract

Heusler alloys based thin-films often exhibit a degree of atomic disorder which leads to the lowering of spin polarization in spintronic devices. We present ab-initio calculations of atomic disorder effects on spin polarization and half-metallicity of Mn₂CoSi inverse Heusler alloy. The five types of disorder in Mn₂CoSi have been proposed and investigated in detail. The A_{2a}-type and B2-type disorders destroy the half-metallicity whereas it sustains for all disorders concentrations in DO_{3a}- and A_{2b}-type disorder and for smallest disorder concentration studied in DO_{3b}-type disorder. Lower formation energy/atom for A_{2b}-type disorder than other four disorders in Mn₂CoSi advocates the stability of this disorder. The total magnetic moment shows a strong dependence on the disorder and the change in chemical environment. The 100% spin polarization even in the presence of disorders explicitly supports that these disorders shall not hinder the use of Mn₂CoSi inverse Heusler alloy in device applications.

Keywords — DFT, disorder, half-metallicity, Heusler alloys