Theoretical investigations of Co2Mn1-xCrxSn and Co2MnSn1-ySiy pseudo-ternary alloys: First principles calculations

Abstract

The electronic and magnetic properties of Co2Mn1-xCrxSn and Co2MnSn1-ySiy alloys are investigated using density functional theory (DFT) within a full-potential linearized augmented-plane-wave (FP-LAPW) method. Amongst the systems under investigation, Co2MnSn1-ySiy alloys show half metallicity with 100% spin polarization at the Fermi level, however Co2Mn1-xCrxSn are found to be pseudo-half metals with few minority states at the Fermi level and high spin polarization. The substitution of Si with Sn keeps the magnetic moment constant in Co2MnSn1-ySiy alloys, whereas the substitution of Mn with Cr decreases the magnetic moment and degrade the half-metallicity in Co2Mn1-xCrxSn alloys. The Curie temperature is calculated and it is found to be about 928 K for all Co2MnSn1-ySiy alloys, whereas it decreases linearly with x for Co2Mn1-xCrxSn alloys. The lattices constants, bulk modulii, energy gaps, polarization ratio and density of states are calculated and their variation versus x or y are discussed.