Structural and optoelectronic properties of NiTiX and CoVX (X = Sb and Sn) half-Heusler compounds: An ab initio study

Abstract

We have performed ab-initio self-consistent calculations using the full-potential linear muffin-tin orbital (FP-LMTO) method to investigate the structural and the electronic properties of some half-Heusler alloys. The local density and generalized gradient approximations were used for NiTiSn and CoVSn alloys. Due to the metallic characters of both NiTiSb and CoVSb compounds, the local spin density approximation was used. Lattice constants, bulk moduli, and the pressure derivatives of the bulk moduli are calculated, band structure and density of states are drawn and effective masses are investigated. To our knowledge this is the first quantitative theoretical prediction of the effective masses for the investigated compounds and still awaits experimental confirmations. The obtained results are agreed well with the other published values.