

Electronic structure, magnetism and robust half-metallicity of new quaternary Heusler alloy FeCrMnSb Heusler alloy

Abstract

A new quaternary Heusler alloy FeCrMnSb is identified by employing ab initio electronic structure calculations. It is stable in Y-structure which is also verified by various conditions governed by elastic constants c_{ij} . It is a true half-metallic (HM) ferromagnet with integer magnetic moment of 2.00 μ_B per formula unit. The values of minority band gap and HM gap are found to be 0.65 eV and 0.1 eV, respectively. The HM character of FeCrMnSb sustains for 6% to 9% of uniform strain and 9% to 12% of tetragonal strain. This new quaternary Heusler alloy can be proved as an ideal candidate for spin valves and magnetic tunnel junction applications (MTJs).

Keywords — Ab initio calculations, half-metallic ferromagnetism, Quaternary Heusler alloys