

A First-Principles Study of Half-Metallic Ferrimagnetism in Ti2FeZ (Z=Al, Ga, In) Heusler Alloys.

Abstract:

Using density functional theory with the full potential-linearized augmented plane wave (FPLAPW) method, we study the structural, electronic and magnetic properties of Ti2FeZ

(Z = Al, Ga, In) alloys with Hg2CuTi-kind alloys structure. These are half-metallic ferrimagnets. In addition to this, the total magnetic moments of Heusler alloys are Ti2FeZ agree with the rule *Mtot* = *Ztot-18* Slater-Pauling with a gap energy 0.56, 0.60 and 0.64 eV in the spin down channel, respectively.

Contribution: Invited