Abstract

The structural, electronic, magnetic, elastic and thermodynamic properties of full Heusler compounds X_2ScGa (X=Mo,Ru,Os) have been investigated in $L2_1$ type cubic structure using first principle calculations using Density Functional Theory (DFT). The electronic band structures, total and partial density of states have been calculated. The calculated band structures confirm the metallic nature of the alloys X_2ScGa (X=Mo,Ru,Os), as valence and conduction bands are overlapping at the Fermi level. The TDOS and PDOS demonstrate that these compounds have metallic characteristics. The calculated mechanical properties reveal that alloys have brittle nature with high stiffness. Magnetic properties show the diamagnetic behavior of the compounds as the net magnetic moment is zero. Furthermore the alloys were examined thermodynamically by using the quasi harmonic approximation with 0–500 K temperature range. These alloys are a possible contender for the iron and steel sectors, according to the findings.