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First Principles Calculations of Co_2FeAl and Fe_2CoAl Heusler Alloys

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Abstract

Ternary intermetallic alloys with X_2YZ stoichiometric composition are known as full Heusler alloys where X and Y are transition elements and Z is p type element. These materials have attracted attention due to several applications such as half-metallicity, ferromagnetism, magnetocaloric, magneto optical, thermoelectric properties, ferromagnetic shape memory, spintronic applications, etc. Direct Heusler alloys with space group Fmm (No. 225) crystallize in ordered $L2_1$ structure whereas inverse Heusler alloys with space group F3m (No. 216) crystallize in ordered $C1_b$ structure. The atomic number of atom X is higher than that of Y in $L2_1$ structure whereas opposite trend is followed in $C1_b$ structure. Present work describes an elucidation of the electronic structure, magnetic and elastic properties of $L2_1$ structure of Co_2FeAl and $C1_b$ structure of Fe_2CoAl heusler alloys using density functional theory (DFT) within generalized gradient approximation (GGA). The band structures, density of states and magnetic moment have been calculated. These results indicate the presence of half-metallicity in Co_2FeAl whereas full metallic behaviour in Fe_2CoAl alloys. Both materials satisfy stability criteria in terms of elastic constants and are associated with ductile behaviour based on G/B ratios.

Keywords: *density functional theory, electronic structure, magnetism, elastic properties*