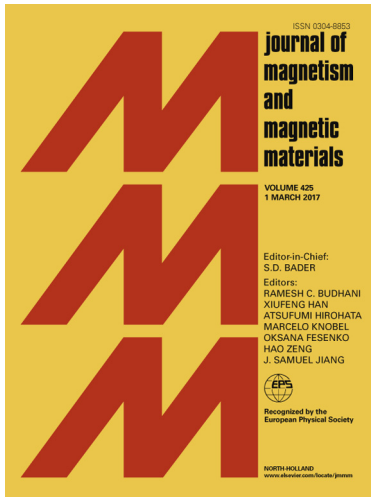

Research articles

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First principles study on Fe based ferromagnetic quaternary Heusler alloys

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Abstract

The study of stable half- metallic ferromagnetic materials is important from various fundamental and application points of view in condensed matter Physics. Structural phase stability, electronic structure, mechanical and magnetic properties of Fe- based quaternary Heusler alloys XX′YZ (X = Co, Ni; X′= Fe; Y = Ti; Z = Si, Ge, As) for three different phases namely α, β and γ phases of LiMgPdSn crystal structure have been studied by density functional theory with generalized gradient approximation formulated by Perdew, Burke and Ernzerhof (GGA- PBE) and the Hubbard formalism (GGA- PBE+U). This work aims to identify the ferromagnetic and half- metallic properties of XX′YZ (X = Co, Ni, X′= Fe ; Y = Ti; Z = Si, Ge, As) quaternary Heusler alloys. The predicted phase stability shows that α – phase is found to be the lowest energy phase at ambient pressure. A pressure-induced structural phase transition is observed in CoFeTiSi, CoFeTiGe, CoFeTiAs, NiFeTiSi, NiFeTiGe and NiFeTiAs at the pressures of 151.6 GPa, 33.7 GPa, 76.4 GPa, 85.3 GPa, 87.7 GPa and 96.5 GPa respectively. The electronic structure reveals that these materials are half metals at normal pressure whereas metals at high pressure. The investigation of electronic structure and magnetic properties are performed to reveal the underlying mechanism of half metallicity. The spin polarized calculations concede that these quaternary Heusler compounds may exhibit the potential candidate in spintronics application. The magnetic moments for these quaternary Heusler alloys in all the three different phases (α, β and γ) are estimated.

Keywords: A. metals and alloys; C. Crystal structure; C. Phase transitions; C. Electronic properties; C. Mechanical properties; D. Computer simulations.

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