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Structural, Electronic and Magnetic Properties of $Ti_{1+x}FeSb$ and $TiFe_{0.75}M_{0.25}Sb$ (M= Ni, Mn) Heusler Alloys SAID AL AZAR, Basic Sciences Department, Dar Al Uloom University, Riyadh, Saudi Arabia, AHMAD MOUSA, Department of Basic Sciences, Middle East University, Amman, Jordan — Density functional theory calculations based on full potential linearized augmented plane-wave (FPLAPW) plus local orbital method in the framework of GGA-PBE, as embodied in the WIEN2k code, is used to investigate the structural, electronic and magnetic properties of intermetallic $Ti_{1+x}FeS$ Heusler compounds, where (x =*i/4, i=-3,-2,-1,0,1,2,3,4*) and the $TiFe_{0.75}M_{0.25}Sb$ (M = Ni, Mn) quaternary semi-Heusler compounds. Moreover, the modified Becke-Johnson exchange potential, as a semi-local method, was employed to predict the band-gap more precisely. We examined the site preference of the parent compound TiFeSb and varying the electron concentration by doping or removing a Ti atom. It is found that they play a crucial role in physical properties of these material systems. The lattice parameters and spin magnetic moment calculated were consistent with the previous experimental and theoretical data available. Moreover, alloys with x<0 are found to exhibit a ferrimagnetic phase, and the alloy with x=0.25 exhibit a non-magnetic properties, whereas the rest have shown ferromagnetic phase. The band-structure analysis of $Ti_{1.75}FeSb$, Ti_2FeSb and $TiFe_{0.75}Ni_{0.25}Sb$ alloys suggested that they could be a ferromagnetic half-metallic members with band-gaps 0.67, 0.41 and 0.54 eV, respectively.

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