ABSTRACT

Materials with diverse physical characteristics, particularly those with a strong connection between spin, lattice, and charge, are required by modern physical world to get competency with less energy consumptions. As a result there is necessity of incorporation of many functionalities into a single material. This thesis focuses on studying the physical characteristics of spintronic optoelectronic and thermoelectric materials in order to propose novel, highly efficient materials for device applications. Half metals have been centered in material science for their wide range applications in spin electronics and future thermal industry due to tunable characteristics. In present work half metallic materials $XFeSe_2$ (X=Li, Na and K) are being computationally focused to study structural, electronic, transport and magnetic properties under the framework of DFT (Density Functional Theory). These first principle calculations extracted from Full Potential Linearized Augmented Plane Wave (FP-LAPW) method. Birch Murnaghan Equation and Predew-Burke-Ernzerhof sol (PBE-sol) scheme within GGA approximation has been used for stability, exchange and correlation potential by Vienna Package WIEN2kwi.Computed parameters of hexagonal structures with space group 164_P-3m1 are in close agreement with ones are reported in literature. Indirect band gap 0.535 eV, 1.127 eV and 0.613 eV is observed in up spin channel reflecting spin polarization around E_F which confirms half metallicity of ternary chalcogenides magnetic semiconductors with magnetic moment $5\mu_B$ per unit cell. Optical explorations of $LiFeSe_2$, $NaFeSe_2$, and $KFeSe_2$ put forward them as an efficient candidates to play role in optoelectronic. Electrical and thermal conductivity, Seebeck coefficient, power factor, and thermal efficiency all are computed and explained in context for thermoelectric nature by using BoltzTraP code in temperature range 0-1000K embedded in DFT. It reveals that these materials would promising materials for thermoelectric applications.