Abstract

Weyl semimetal materials have gained a keen interest to the scientist for their wide applications in the field of magneto-electronics and in spintronics devices due to their "exotic surface states". In this thesis, research work mainly focuses on the theoretical study of Weyl semimetal materials **XCd_2As_2** (X=Eu, Sm and Gd). The theoretical study involves the investigation of structural, electronic, optical, and magnetic properties of Weyl semimetals compound **$EuCd_2As_2$**, **$SmCd_2As_2$** and **$GdCd_2As_2$** under the frame of Density Functional Theory (DFT). These calculations are based on first principle technique within Full Potential Linearized Augmented Plane Wave (FP-LAPW) method. Perdew-Burke-Ernzerhof Generalized Gradient Approximations (PBE-GGA) has been used for the exchange and correlation potential by employing CASTEP-code. Our calculated structural parameters are in good agreement with previous research work. In our study, these compounds have band touching nodes at some symmetry points. The calculated values of band gaps are in good agreement with other theoretical works.

Electronic results reveal that these compounds have band touching nodes at gamma symmetry points. Weyl fermions in these compounds is justified through electronic properties. The calculated values of band gaps are in good agreement with other theoretical data. These compounds confirm large magnetic moment $5.95\mu_B$, $7.01\mu_B$ and $7.67\mu_B$ which is a sign of ferromagnetic material. Basically, these large magnetic moments values occur due to the half-filled f orbitals present in each compound. Also, spin density of states show that up-spin channel is dominant near the gapless surface states which allow single spin channel moment and thus have no hurdle in the way of charge. The optical associated quantities such as the dielectric function, energy loss function, reflectivity, absorption, optical conductivity, and refractive index are also evaluated by ab-initio calculations. Furthermore, a complete study of these compounds shows that they are more suitable for efficient electronics, spintronics and optical devices.