# ABSTRACT

The thesis deals with the electronic band structure calculations of some compounds, namely, metallic compound ($CuS_2$), inter-metallic compounds $Ti_3M$ (M=Au, Pt, Ir) and semi-metallic compounds $Sb_2Te_xSe_{3-x}$ (x=3, 2, 1, 0). The main objective of the present work is to study the associated properties of the above mentioned compounds. The present computational work has been carried out by using the results such as density of states (DOS), equation of states (EOS), Fermi energy ($E_F$) etc., obtained from the first principles electronic band structure computations of these compounds. The ab initio self consistent calculations of electronic band structures have been carried out through the tight binding linear muffin tin orbital (TB-LMTO) technique within the atomic sphere approximation (ASA). Within this method, the electronic band structure calculations are performed for the above mentioned compounds at their equilibrium, compressed and expanded volumes. The electronic total energy values are obtained for various unit cell volumes and fitted to Murnaghan's equation of state to obtain the ground state properties.

The estimation of thermal properties, such as Debye temperature, electronic specific heat co-efficient and superconducting transition temperature and these studies have been carried out by using the results of electronic band structure and related characteristics, for the $CuS_2$ ($FeS_2$-type structure) compound in two different phases, (cubic phase and orthorhombic phase) under pressure. Apart from the electronic band structure and structural stability, the density of states (DOS) and Fermi energies ($E_F$) are also

calculated for various unit cell volumes. The equilibrium ground-state properties were calculated for the lattice parameters that correspond to the minimum of the electronic total energy. From the total energy it has been observed that the cubic phase is the stable phase under normal pressure. The result indicates that, in both the phases of the material, the p-bands dominate in their conduction band. The DOS around $E_F$ is found to be high and it is due to the strong pile up of mainly the p-states and a little of d-states, in both the phases of $CuS_{2,}$ and accounts for the structural stability. Thus, the DOS at the Fermi level is almost exclusive of p-character. The Debye temperature ($\theta_D$) and electronic specific heat co-efficient ($\gamma$) are important parameters that are closely related to the thermal properties of materials. The electron-phonon coupling constant ($\lambda$) and superconducting transition temperature ($T_C$) has also been carried out for pyrite structure $CuS_2$ compound.

Ti-based A15-structured compounds $Ti_3Au$, $Ti_3Pt$, and $Ti_3Ir$ are interesting due to their thermal and superconducting properties. The basic electronic properties of these materials have been computed and, the results have been used for the studies of electronic ground-state, thermal and superconducting properties of the compounds $Ti_3Au$, $Ti_3Pt$, and $Ti_3Ir$. The total energies are calculated as a function of primitive cell volume for all the above-mentioned compounds, and are fitted to the Birch equation of state (EOS) to obtain the ground-state properties, such as equilibrium lattice constants, bulk modulus, cohesive energy and heat of formation. The obtained results are compared with the available experimental and other theoretical results. The domination of p- and d-bands is clearly evident in all the three materials. They are also found to be very strongly hybridized. The band structures show that the Fermi energy decreases with the decrease in the atomic number of M (M=Au, Pt, Ir) element. The DOS at the Fermi level is

observed to be almost exclusively of d-character with little contribution from p-bands. The cohesive energy, heat of formation, Debye temperature ($\theta_D$) and Grunesian constant ($\gamma_G$) of $Ti_3Au$, $Ti_3Pt$, and $Ti_3Ir$ compounds has been computed. The electron-phonon coupling parameter $\lambda$ has been estimated using the electronic band structure results and the superconducting transition temperature $T_C$ is calculated. The $T_C$ values estimated by the present work for all the three compounds, $Ti_3Au$, $Ti_3Pt$, and $Ti_3Ir$, are found to agree reasonably with the available experimental values.

The details of studies and results of $Sb_2Te_xSe_{3-x}$ (x=3,2,1,0) compounds, such as $Sb_2Te_3$, $Sb_2Te_2Se$, $Sb_2TeSe_2$ and $Sb_2Se_3$ regarding their electronic structure, density of states, band gap, Fermi energy and Debye temperature have been computed for all these antimony compounds and the results are corroborated well with the earlier experimental reports. The bulk modulus $B_0$ is used to obtain the Debye temperature ($\theta_D$) for the three trigonal systems ($Sb_2Te_3$, $Sb_2Te_2Se$ and $Sb_2TeSe_2$) and one orthorhombic structure ($Sb_2Se_3$). The Debye temperature ($\theta_D$) values obtained here are found to be in close agreement with the available experimental results. The studies further reveal that the electronic properties are highly dominated by the p-orbitals originating mainly from Sb. Semi-metallic nature of all the four compounds is clearly displayed in their band structure and density of states results. The energy gap and density of states at $E_F$ increase as Se content increases for all the compounds; however, the Fermi energy and bulk modulus values increases with the increases of Se content from $Sb_2Te_3$ to $Sb_2TeSe_2$, and then they decreases considerably for $Sb_2Se_3$. Such a drastic change of these of these properties for $Sb_2Se_3$ is attributed to the structural phase change from trigonal to orthorhombic structure.

The present work thus comprises the computation of electronic band structure properties and the electronic total energy calculations as a function of volume for the compounds viz., transition metal dichalcogenide pyrite structure compound copper disulphide ($CuS_2$), A15 structure of binary $A_3B$ type inter-metallic compounds $Ti_3M$ (M=Au, pt, Ir) and semi-metallic (V-VI) layered (antimony telluride, antimony selenide ditelluride, diantimony telluride diselenide, antimony selenide ) $Sb_2Te_xSe_{3-x}$ (x= 3,2,1,0) compounds. These band structure results have been, inturn, used to carry out studies on structural, thermal, and superconducting properties of these materials. The computed results are found to corroborate satisfactorily the literature. The studies, hence, have provided a comprehensive understanding of the fundamental aspects of these materials.