CHAPTER 7

CONCLUSIONS

This chapter contains the conclusive remarks on the outcome of the research conducted and presented in this thesis.

The self-consistent TB-LMTO method has been employed in order to study the structural, electronic, thermal, and superconducting properties of some of the compounds, namely, 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, the total energy calculations were performed, based on the density functional formalism within the framework of the LDA and ASA.

Band structure calculations have served as a powerful tool in bringing out successfully the connection between microscopic atomistic properties, such as the wave functions with several macroscopic superconducting properties of a large number of intermetallic compounds for which they have been applied.

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 (θ_D) and electronic specific co-efficient (γ) are important parameters that are closely related to the thermal properties of materials. The electron-phonon coupling constant (λ) 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. The cohesive energy, heat of formation, Debye temperature (θ_D) and Grunesian constant (γ_G) of Ti_3Au, Ti_3Pt, and Ti_3Ir compounds has been computed. The electron-phonon coupling parameter λ 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 (θ_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 (θ_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, in turn, 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.

The results obtained in the present calculations indicate, that the total energies calculated using the DFT within the LDA are sufficient to predict the metallicity, structural phase stability and the ground-state properties in these compounds. Several predictions are made in the present work. This work may be further extended to predict the superconducting property of different structures, and to calculate the optical, thermal and magnetic properties.