CHAPTER 7: OVERALL CONCLUSION AND OUTLOOK

In this thesis, we have reported a complete study on the structural phase transition, elastic properties and electronic properties of Group III-V (GaP, GaAs, InP, InAs) and Group II-VI (ZnS, CdTe and ZnSe) compound semiconductors in both zinc blende (ZB) and rock salt (RS) structures. We have also studied the effect of InP doped with Ga: $In_xGa_{(1-x)}P$ alloy at different concentration of Ga. The major outcome of this wok can be summarized as

A. Group III-V Compound semiconductors

The structural properties of GaP, GaAs, InP and InAs has been studied in both zinc blende (ZB) and rock salt (RS) structures. The structural phase transformation from ZB to RS phase under induce pressure for GaP, GaAs, InP and InAs are found to occur at 21.9 GPa pressure with a volume collapse of 14.11%, 10.7 GPa pressure with a volume collapse of 14.2%, 9.3 GPa pressure with a volume collapse of 16.45% and 4.7 GPa pressure with a volume collapse of 17.2% respectively.

The elastic constants (C_{11}, C_{12} and C_{44}) of both the ZB and RS phases of these compounds are found to satisfy the mechanical stability conditions and undergo a linear variation with increase in pressure. The elastic parameters (Zener Anisotropy factor (A), Poisson's ratio (υ), Kleinmann parameter (ζ), B/G ratio, Young's modulus (Y) and Deby's temperature (θ_D) are also calculated.

The energy band structures for GaP, GaAs, InP and InAs (in both the phases) at zero pressure as well as under induced pressures are studied within the LDA, GGA and mBJ-GGA. At zero GPa pressure, we find that calculation within the mBJ-GGA gives us better results (energy band gaps) than the LDA and GGA methods. The ZB structures of GaP is found to be an indirect band gap semiconductor with band gap of 2.33 eV while GaAs, InP, InAs show a direct

energy band gap of 1.3 eV, 1.31 eV and 0.35 eV respectively. The RS structures of the above semiconductor compounds are found to be metallic without much variation under induced pressure.

Further analysis in the band structure of the ZB phase of these semiconductor compound shows an increase in the energy band gap between the Γ-L point and a decrease between Γ-X point towards the Fermi level with increasing pressure indicating possibilities of shifting of the energy bands and crossing over of the conduction band towards the valance band confirming the metallic nature of GaP, GaAs, InP and InAs after structural transformation to the RS phase.

B. Group II-VI compound semiconductors

Following similar trend as in chapter 4, the structural properties, elastic properties and phase transformation from the ZB to RS structure under induced pressure for ZnS, CdTe and ZnSe are studied. We find that the above semiconductor compounds undergo a phase transition from ZB to RS at 17.6 GPa pressure with a volume collapse of 12.86%, 4.0 GPa pressure with a volume collapse of 20.9% and 11.5 GPa pressure with a volume collapse and 13.74% respectively.

The energy band structures study of the ZB phase shows a direct band gap of 1.46 eV, 3.5 eV and 2.5 eV in case of ZnS, CdTe and ZnSe respectively. RS phase for CdTe and ZnSe show a metallic character while ZnS (RS phase) shows an indirect band gap.

We find that implementation of the mBJ-GGA potential in the energy band gap calculation resolves the underestimation of the band gaps with LDA, GGA and provides better results closer to the experimental value while study of the energy band gap under induced pressures reveals that the energy band gap of ZB phases are affected by pressure while the energy band gaps of the RS phases are not much affected by pressure.

C. Effect of Doping: InP doped with Ga ($In_xGa_{(1-x)}P$)

Understanding the doping effect in the compound semiconductors is very important to see the possibility of tailoring physical properties and electronic structure. The structural phase stability from the zinc blende to rock salt structure and electronic structure of $In_{1-x}Ga_{1-x}P$ has been performed to understand the doping effect of Ga in InP compound semiconductor. The lattice parameters of the stable structures of the corresponding doping concentrations are compared with other available theoretical and experimental results and found to be in good agreement with them. The composition effect on the lattice constant, bulk modulus and the formation energy are studied at different concentration of x (= 0.0, 0.25, 0.5, 0.75, 1) for both zinc blende and rock salt structure. The phase transition pressure from zinc blende to rock salt phase in different concentration is found to increase with increase in concentration of Ga. The electronic band structure at different concentration of 'x' has been investigated using the total and partial density of states. The study on the energy band gap of zinc blende phase of $In_{1-x}Ga_xP$ alloy shows a non-linear behaviour with concentration. The direct energy band gap of InP increases as the concentration of Ga atom increases upto 0.25. After that it starts decreasing with concentration (x=0.5, 0.75) and finally change to an indirect band gap of GaP at x=1.0. The DOS study shows an increase in energy band gap in lower concentration of Ga while increase concentration of Ga atom leads to a decrease in the energy band gap. The rock salt phase of $In_{1-x}Ga_xP$ alloy at different concentration of 'x' shows crossing over of the conduction band and the valance band at the Fermi energy thus showing metallic character of the $In_{1-x}Ga_xP$ alloy at all the concentrations of 'x'.

Hence our study constitute a preliminary step to future work dealing with super lattices, complex system semiconductors. It will stimulate experimental studies of high pressures and shed new light on high pressure application of optoelectronic devices.