7.1 Summary and Conclusions

This last chapter of the thesis summarizes briefly, the entire work of present study along with the important conclusions emerging. Wherever possible this chapter also highlights the scope of the extension of the study for further investigations.

The present work of the thesis is computational in nature. To study various electronic, elastic and thermodynamic properties of the crystal, several different approaches like pseudopotential method, dielectric two-band model, full potential linearized augmented plane wave method, tight-binding method, self-consistent method using local-density-functional approximation (LDA) and generalized-gradient approximations (GGA) in density functional theory, ab initio method etc. have been successfully used by many people [1-16]. Out of all these methods, the pseudopotential theory is the simplest method dealing with the physical properties of alloys and compounds of semiconductors; hence it is used with its local model potential form in the present work [1, 16].

The proper characterization of the pseudopotential is essentially required before making any theoretical application to semiconductors. The potential should be capable to compute various atomic, dynamic, static, vibrational, electronic and magnetic properties with good precision. For this we have proposed a model potential bearing a single parameter in the real space [1]. To represent core-core repulsion usually Born-Mayer term is employed. We have also incorporated this feature in our potential through exponential factor. Inside the core, it is represented as the combination of linear and quadratic terms modulated by repulsive exponential factor, which tends to cancel Coulomb potential inside the core. While outside the core, it has the Coulombian tail. It becomes analytic at $r = 0$ and smoothness of the bare-ion potential due to exponential term results into faster convergence in $r$-space. In addition, this bare-ion potential is continuous at the core. Thus the model potential has the novel feature of representing varying cancellation of potential within the core over and above its continuity and weak effect. The model potential is simple and convenient to use.
as it has only one parameter, the pseudocore radius. The form factor satisfy the required limiting values at \( q \to 0 \), \( W(q) \to -2/3 \) \( E_F \) and at large \( q \), present model potential is free from any abnormal or unwanted oscillations which is highly desirable for any pseudopotential formalism.

To characterize this model potential we opted zero pressure or equilibrium method [16] as it is free from any fitting with the experimental results and more meaningful in nature. By using zero-pressure condition we have determined the value of the parameter of the potential. However, this method depends on the choice of local field correction function; we have incorporated six different screening functions due to Hartree [17], Taylor [18], Ichimaru et al. [19], Farid et al. [20] and Sarkar et al. [21] along with new and less explored screening function due to Nagy [22]. The most recent Nagy’s static local field correction function [22], which is first time preferred for all semiconducting materials, is a static local field correction function derived from a model pair-correlation function for a dense electron gas.

In the present work, We have used higher order pseudopotential theory to study various physical properties of semiconductors of group IV, their binary alloys, group III-V and II-VI semiconductor compounds, ternary alloys and quaternary alloys theoretically.

Following are some important conclusions emerging from the entire work carried out during the present investigations.

- The proposed form of model potential can be used extensively to calculate total energy, energy-volume relations, pressure-volume relations (equation of states), bulk modulus, bulk modulus-volume relations, bulk modulus-pressure relations, pressure derivative of bulk modulus, elastic constants, Young modulus, shear modulus, Poisson’s ratio, sound velocities of longitudinal and transverse waves in \([1 0 0]\), \([1 1 0]\) and \([1 1 1]\) directions, energy band gap at Jones-zone face, variation of energy band gap at Jones-zone face with volume and pressure of group IV semiconductors, group III-V and II-VI semiconductor compounds, optical properties like refractive index,
plasmon energy, electronic polarizability, bond length etc. of semiconductors. Along with these properties it can be applied to compute heat of formation, ratio of heat of formation, phase diagram at low temperature and at melting temperature, the Helmholtz free energy of formation of solid solutions or alloys. The parameter of the potential is derived from equilibrium condition that is zero-pressure condition, not fitting with any experimental data.

- Nagy’s local field correction function [22] is successfully incorporated in such type of extensive work for semiconductors and it gives good results for almost all properties under consideration.
- The results of total energy computed by the proposed model potential [1] are in good agreement with the available experimental findings and other such theoretical data.
- The equation of states computed by present approach is agreeing with those computed by Murnaghan [23] and Vinet’s formulations [24] with some deviation at high compression.
- The present results of bulk modulus, elastic constants, Young modulus, shear modulus and Poisson’s ratio are satisfactorily agreeing with the experimental findings and other such theoretical results.
- Some underestimation is observed for pressure derivative of bulk modulus.
- To determine elastic constants, we have used symmetric and antisymmetric part of the potential only at one point (1 1 1), which create small deviation in elastic properties of some semiconductors under consideration.
- The present findings of wave velocities of longitudinal acoustic waves and transverse acoustic waves along [1 0 0], [1 1 0] and [1 1 1] directions are excellent.
- The present findings of energy band gap at point X on the Jones-zone face are satisfactorily agreeing with the experimental and other theoretical findings.
- The refractive index computed from energy band gap at point X on the Jones-zone face for group IV, group III-V and II-VI semiconductors are computed using nine different relations. Some deviation is seen for group IV semiconductors. But good agreement is achieved for group III-V and II-VI semiconductors.
semiconductors. To the best of our knowledge, we are reporting first time the computation of refractive index with different screening functions.

- We have obtained excellent agreement of the present findings of some optical properties like high frequency dielectric constant, bond length, electronic polarizability, plasmon energy with the experimental results and other theoretical results. In some cases the present results are better than other such theoretical results.

- For ternary and quaternary semiconductors, very limited experimental data or other theoretical data for the properties under investigation are available for comparison. Present work also provides a good reference for comparison of theoretical and experimental results.

Some of the future scope for further investigations in the field of semiconductors are given below.

- The present approach can be extended to study different properties of pentanary alloys.
- The magnetic properties of some magnetic semiconductors can be predicted by using the same approach.
- In the present work we have considered only diamond or zinc-blende phase for the computation of certain properties of semiconductors. This approach can be used extensively for hcp, rocksalt, wurtzite structures or some disordered materials too.
- The work can be extended to compute various properties of liquid semiconductors.
- The phonon related properties, phonon dispersion curves and thermodynamic properties can be predicted using this theoretical model.
- The band structure may be calculated by using present model with some modifications.

Thus, our proposed model potential can be used to compute many properties of semiconductors having different phases and states to accomplish a comprehensive study.
7.2 References