Chapter 7

Conclusions and Future scope


7.1 Conclusions

This thesis is devoted to the study of electronic and structural properties of binary and ternary III-V and II-VI compounds using LCAO method as implemented in the CRYSTAL06 code. The structural properties are interpreted in the terms of lattice constants, transition pressure, bulk modulus and its pressure derivatives whereas the electronic properties in terms of cohesive energy, energy bands, momentum density and bonding in these systems.

In case of III-V compounds, the structural and electronic properties of AlX (X=N, P and As) compounds have been reported. The computed results are compared with the previous experimental and theoretical results. This investigation suggests that the AlP and AlAs becomes metallic under pressure.

The ground state properties of II-VI compounds i.e SrO, SrS, BeS, BeSe and BeTe have been presented. In case of SrO and SrS, structural phase transition and energy band have been reported. These compounds changes from B1 to B2 phase at pressure of about 18.4 GPa. The calculated results are in good agreement with the earlier experimental values.

The structural, optical and electronic properties of BeX compounds have been investigated. This study suggests that these compounds have indirect band gaps. In addition, the effect of pressure on electronic and optical properties of BeS is also studied. It is observed that the dielectric constant and indirect band gap increases and decreases with pressure respectively. On the basis of EVED profiles, it is found that BeTe is more covalent and less ionic than BeS and BeSe.

The electronic properties of Mg$_x$Ca$_{1-x}$O (x = 0.0, 0.25, 0.50, 0.75, 1.0) have been calculated. The electronic properties are explained in terms of band structures, DOS, anisotropies in momentum density and EVED profiles. The analysis of these properties indicates that the band gaps at the equilibrium lattice constant increases with the increasing Mg concentration.
The overall results are in good agreement with the previous reported experimental and theoretical values. Thus, it is concluded that LCAO calculations can be used for the better understanding of crystalline compounds.

### 7.2 Future scope

Although, the investigations carried out on these materials have systematically outlined some important features related with electronic structure, electron momentum distribution, phase transition, dielectric constant, some obvious suggestions can be given as follows:

a) The present results are only the prediction of the ground state properties of solids. Therefore, the experimental analysis is needed to examine the computed values.

b) This study also stimulates to investigate the electronic and structural properties of these compounds using the newly developed exchange and correlation functionals.

c) The present investigations on Mg$_x$Ca$_{1-x}$O alloys show the modifications in ground state properties. Hence, the transition element doping in MgO or CaO can also be done in order to see the magnetic properties in this system.

It is hoped that this work will stimulate further studies in the field of condensed matter and high pressure physics.