The thesis deals with the calculation of the electronic band structure and superconductivity of elemental solids Te and Se in their high pressure bcc phase. The structural phase transition and insulator to metal transition in some of the alkaline-earth chalcogenides namely BaS, BaSe, BaTe, MgO, CaO and SrO and the structural and electronic properties of the alkaline-earth fluorohalides CaFCl, SrFCl, BaFCl, BaFBr and BaFI have been studied. In addition other physical properties such as electronic specific heat coefficient and the electrical resistivity of elemental solids have been calculated.

The conventional linear muffin-tin orbital method (LMTO) is used to obtain the electronic band structure of elemental solids and for the compounds tight-binding linear muffin-tin orbital method (TB-LMTO) is used. The superconducting transition temperature (T_c) of the elemental solids were calculated using McMillan's formula. The total energies in the framework of density functional formalism within the local density approximation were used in determining the structural phase transition of the compounds.

The group VIb elements Te and Se at ambient conditions crystallize in the hexagonal structure with spiral chain arrangement and are semiconductors. Both Te and Se are known to exhibit a sequence of structural phase transitions under pressure. The high pressure phases are metallic and are found to be superconducting at low temperatures. The latest known high pressure phase for both the elements is the bcc phase. Recently the T_c of Te and Se were measured as a function of pressure. For
Te the $T_c$ measurements were made upto the bcc phase, whereas for Se the $T_c$ measurements were limited to the low pressure region.

To explain the superconducting behaviour of bcc Te and Se, the electronic band structure of these elements in their bcc phase were obtained as a function of pressure. The calculated lattice constant and the pressure volume (P-V) relation are found to be in good agreement with the experimental values. The band structure outputs were used to calculate the $T_c$. The calculated value of $T_c$ of Te in the bcc phase is 7.2 K which decreases with pressure. This is in agreement with the experimental observations for both magnitude and trend. In the case of bcc Se, we predict the value of $T_c$ to be 2.3 K which decreases with pressure. The decreasing trend in the $T_c$ values is a typical behaviour of $sp$ metals. Also the electrical resistivity ($\rho$) has been calculated for both the elements which is found to decrease with pressure. The negative value of $dT_c/dp$ and $d\rho/dp$ is due to the stiffening of the lattice upon compression.

The alkaline-earth chalcogenides BaS, BaSe, BaTe, MgO, CaO and SrO which are being studied in the present work crystallize in the NaCl-type (B1) structure at ambient conditions. Except MgO all the other systems that are being studied are experimentally found to undergo structural phase transition to the CsCl-type (B2) structure under pressure. Apart from the B1-B2 structural phase transition, barium chalcogenides are found to exhibit the interesting phenomenon of metallization upon further compression in their B2 phase.

The self-consistent scalar-relativistic band structures of BaS, BaSe and BaTe were obtained in the B1 and B2 structures at equilibrium volume as well in the high pressure region. The total energies were calculated as a
function of reduced volume and fitted to the Birch equation of state (EOS) to obtain the equilibrium lattice constant, bulk modulus, P-V relation and the enthalpy. The calculated ground state properties and the B1-B2 structural transition pressure, were found to be in good agreement with the experimental values.

These compounds are found to be indirect band gap semiconductors with band gap occurring between $\Gamma$ and X-points. The calculated values of band gap in the B1 structure are found to be underestimated by 30 - 40%. In the B2 structure upon further compression the band gap decreases leading to the overlap of the valence and the conduction bands. The calculated values of metallization volume and pressure in the B2 structure are lower than the experimental values. This order of error arises due to the use of LDA to the exchange-correlation part of the potential.

The B1-B2 structural phase transition and the effect of compression on the band gap have been calculated for MgO, CaO and SrO. The calculations were performed similar to those of barium chalcogenides. The calculated ground state properties were found to be in good agreement with the experimental values. For MgO, we predict the B1-B2 structural transition to occur around 1975 kbar. The calculated values of transition pressure for CaO and SrO are in agreement with the experimental values.

CaO and SrO are found to be indirect band gap semiconductors with gap occurring between $\Gamma$ and X-points, whereas MgO is a direct band gap semiconductor with gap occurring between $\Gamma$-points. At ambient conditions the band gap values are found to be underestimated by 30-40% when compared to the experimental values. This is the general trend observed while working with LDA. On compression the direct band gap at $\Gamma$ in MgO
increases whereas the indirect band gap in CaO and SrO decreases. At nearly 40% compression, the band gap values in CaO and SrO are 2.2 eV and 2.0 eV, which indicates that there is a possibility of metallization in these two compounds at further high pressure. In MgO the gap at about 45% compression is 6.3 eV, which shows that metallization may be possible only at ultra high pressures.

The alkaline-earth fluorohalides CaFCl, SrFCl, BaFCl, BaFBr and BaFI studied here, crystallize in the tetragonal PbFCl-type structure. These compounds activated with divalent impurities are used as x-ray phosphors in image plates. The structural and electronic properties of these compounds have been studied. The electronic band structure presented here are the first ever calculations performed for these systems.

The total energies for each of the compounds were calculated both as a function of reduced volume and c/a ratio. The calculated total energies as a function of volume were fitted to the Birch EOS to obtain the ground state properties. The calculated equilibrium lattice constant, c/a ratio and the P-V curves were found to be in good agreement with the experimental values.

These compounds are found to be direct band gap semiconductors with gap occurring between Γ-points. The calculated values of band gap are found to vary from 5 to 8 eV which is typical of other alkaline-earth halides. The band gap values for these compounds are not available for comparison except for BaFBr for which it is 26% less than the experimental value. Upon compression, the direct band gap at Γ increases initially and then starts decreasing leading to metallization at high pressures.