

#### 1.1 General introduction

Semiconductor devices play a key role in modern technologies for example solar cells [1], light emitting diodes[2], radiation detectors [3], high temperature electronics[4] etc. The operating conditions of a device depend primarily upon the forbidden energy gap of material used in its fabrication. Conventional semiconductors like silicon have been dominating candidate in the semiconductor industry since the invention of silicon based integrated circuits. But with increasing demand in modern technologies, it has become challengeable to extract additional performance from Silicon based devices due to their low band gap (1.1 eV).

Wide band gap semiconductors become a hotspot of modern semiconductor technology with the ability of working efficiently at high temperature /power, high radiation and harsh environmental conditions. Among a vast range of semiconductors group III -V (AX, A=Al, Ga, In, B; X=N, P) and II-VI (BY, B=Be, Mg, Cd ; Y=O, S, Se, Te) compound semiconductors constitute a specific subgroup of wide band gap semiconductor [5]. These materials form a host material system for the fabrication of devices having numerous significant applications in both civil military fields [6]. These devices can be categorized as electronic and optoelectronic devices. For military electronic equipments, the semiconducting components must have the high reliability to operate in harsh environment of high temperature and high radiations [7]. Thanks to their wider band gap, III-N especially GaN have been most successful in the fabrications of next generation military electronic equipments. The development of solar blind ultraviolet photo detectors, green and blue light emitting diodes are some more fields of applications of III-V and II-VI compound semiconductors, which enjoy the benefit of wider band gap of these materials [6]. In addition to this, III-nitride devices are expected to operate adequately in high temperature conditions and hence can be used without the requirement of any cooling system. This reduces the cost and weight of the resulting systems. The recent thrust area for research in the field of III-V and II-VI material includes the development of laser diodes emitting the radiations in

short wavelength range extending from ultraviolet to green spectral region [6, 7]. For example III- nitride compound semiconductors have been developed for fabricating blue light emitting diodes[8, 9].The shorter wavelength of laser diodes enables the beam to focus in smaller spot. This helps in increasing the storage capacity of optical medium [6].

By alloying the other elements from the constituent group in host material the optical and structural properties of the material can be tuned for desired potential applications [10, 11]. Thus for designing new materials and tailoring them for desired optical applications, we need a fast and accurate determination of their optoelectronic properties. The optical response of a material depends solely upon the interaction of oscillating electric field of incident radiations with electrons of the target system. Thus the electronic structure has to be explored first, in order to study the optical behaviour of a substance. The calculation of properties of proposed materials using first principle based computational methods provides an efficient way for the experimentalists to predict optical and electronic properties prior to their synthesis.

The first principle description of the electronic structure of a solid is a many body problem which requires the solution of quantum mechanical Schrodinger wave equation for the electrons and atomic nuclei. The large mass of the atomic nucleus as compared to that of electron allows the separation of the electronic motion from that of nuclei [12]. As a consequence the problem is reduced to solving the Schrodinger equation for electrons only, subject to an effective potential produced by the nuclei and other electrons. In DFT, instead of using the many electrons wave function which depends upon  $3N$  coordinates of an  $N$  electron system, the electron ground state density is used as the central quantity [13]. The electron ground state density, being a function of three coordinates only, is much simpler as compared to the wave function. In principle, ground state density includes all the information of the system. The problem is further simplified by introduction of two theorems proposed by Hohenberg and Kohn [12]. According to the first theorem, the external potential experienced by each electron can be uniquely expressed as a functional of exact ground state density. As a consequence the expectation value of every observable and hence of Hamiltonian or total energy can be expressed as a unique functional of ground state density. However, the exact ground state is not known prior. Here the second Hohenberg and Kohn theorem plays a role by postulating that total energy attains a minimum value for the

exact ground state density. This allows using the variational principle for minimising the total energy of the system with respect to the electron density [12].

In order to get the exact ground state density to find the functional dependence of total energy on electron density, Kohn and Sham proposed an auxiliary system of non interacting electrons known as Kohn and Sham system. The effective potential of Kohn and Sham system is adjusted in such a way that the ground state electron density of real interacting system of electrons coincides with that of non interacting system of electrons [13]. In KS scheme total energy of the system can be expressed as the sum of kinetic energy of non interacting electrons, the Hartree energy and exchange correlation energy. The last term arises due to the difference between the real system and the non interacting electron gas. Thus, for obtaining the total energy as a functional of electron density we have to find all the three contribution accurately. Unfortunately exact form of the exchange correlation energy is not known. So we have to approximate its value which results in a compromise with the accuracy of the method.

In its simplest form XC functional can be obtained from the so-called local density approximation (LDA) [14] which depends only on the electron density. Since in most of the real systems, there exist in homogeneity in the electron density. So one have to take into account the effect of the densities of neighbouring volumes also, while calculating the exchange correlation energy of a particular volume element. This is done in, so called, Generalized Gradient Approximation (GGA) [15, 16], which includes the gradient of the electron density as well in the expression for XC functional. As a consequence of freedom in incorporating the gradient of density in XC functional, several versions of GGA are possible e.g. PBE [16], WC [17], PBEsol [18] etc. Each of these functionals has their own specific area of validity in producing accurate results. None of the functional produces the accurate results for all types of properties of a given class of materials. A simplest way to select a proper functional is to make a testing of a number of approximations which is based upon the comparison with the experimental results. In our present work we made a testing of different XC functionals (like LDA [14], PBE [15, 16], WC [17], PBEsol [18], SCAN [19], TBmBJ [20]) lying on the first three rungs of the Jacob's ladder [21] by calculating the electronic and optical properties of II-VI and III-V binary compound semiconductors. Before preceding further, a brief introduction to the materials included in our study have been made.

Semiconductors may be classified as elemental or compound semiconductors depending upon whether the crystal is formed by atoms from a single element or from a number of elements. The compound semiconductors are generally obtained by forming solid state solutions of elements taking from Group II to VI of the periodic table. In order to form the solid solutions the two species should have similar valencies, comparable atomic radii and electro negativity in addition to almost similar crystal structures. A compound semiconductor with the general formula of  $A^N B^{8-N}$  where N is the valency of atom A, represents a binary compound semiconductor. By alloying other elements ternary (e.g. AlGaAs), quaternary (e.g. InGaAlP) and higher order compound semiconductors can also be prepared [3]. However in the present work, we focused our study on the binary compound semiconductors only e.g. group III-V and II-VI semiconductors.

Group III-V semiconductors are compound semiconductors formed by combining a cation from group III (e.g. Al, B, Ga, In) with an anion from a group V (e.g. N or P). Although the two ions are covalently bonded, a component of ionic bonding also exists in these substances. This ionic character in the bonding is due to difference in their electro-negativity. Group III-nitrides is a common name given to Aluminium Nitride (AlN), Gallium Nitride (GaN), Indium Nitride (InN) and their alloys [6]. Similarly when group III cation combines with Phosphorous ion, the resulting compound formed is known as III-phosphide. The exceptional properties like wide band gap make these materials the ideal building blocks for a variety of electronic and optoelectronic devices [6]. The exceptional interest in these materials is driven by their potential for electronic and optoelectronic device applications[5]. Group III-N can have three different crystalline structure i.e. the hexagonal wurtzite, cubic zinc blende and rock salt. Under ambient conditions the hexagonal wurtzite structure [22] is most stable phase for all the nitrides except BN, while there are reports for stabilization in zinc blende structure when thin films are grown on cubic substrate using epitaxial growth techniques [22]. For boron nitride zinc blende structure is thermodynamically most stable face under ambient conditions, unlike the other nitrides [22]. Under high pressure conditions all the nitrides transform to the rock salt face. Wurtzite structure can be considered to consist of two hexagonal sub lattices interpenetrating each other with one displaced relative to the other by a cell height  $5c/8$  along c-axis of the hexagonal unit cell. Each of the sub lattice is occupied by one type of the atom. In zinc

blende structure with space group 216 ( $P6_3mc$ ) in Hermann Mauguin notation, each lattice point of cubic unit cell is occupied by two atoms with one having the coordinates  $(1/4, 1/4, 1/4)$  relative to the other. In both zinc blende and wurtzite structure, each atom is surrounded by four other similar atoms lying at the corners of a regular tetrahedron. Thus every atom exists at the centre of a regular tetrahedron with four other atoms at the corners. In rock salt structure each atom is surrounded by six other similar type of the atoms. Hence in wurtzite conventional unit cell there exist six atoms of each type, in zinc blende each unit cell carry four atom while rock salt unit cell six atom of each type. Gallium Nitride is reported as a direct band gap semiconductor in wurtzite and zinc blende structure with zero temperature band gap of 3.510 eV [5]. On the other hand Aluminium Nitride is a direct band gap semiconductor with a larger gap value of 6.23 eV at low temperature, however in zinc blende phase have an indirect band gap of 5.4 eV [5]. In case of InN an unusual variation in the reported values of band gap have been observed. Earlier studies on absorption spectrum of sputtered thin films provided a band gap of 1.7 to 2.2 eV range [5]. Photoluminescence study by Wu et. al. [23] reported a band gap of 0.7 to 0.8 eV lower than the early observation. The recommended value for InN band gap in wurtzite structure is 0.78 eV by Vurgaftman et. al. [5]. There are a number of reports indicating the wrong estimation of metallic character for InN in both wurtzite and zinc blende phase by local and semi local functionals [24, 25]. However applications of recently proposed exchange potential by Tran and Blaha have modified the band gap up to 0.62 eV and 0.76 eV [24].

Under ambient conditions, unlike III-N, III-phosphides (AlP, BP, GaP, InP) are stable in zinc blende phase with space group  $F_43m$  with face centered cubic lattice. GaP and AlP are reported as semiconductors with indirect band gaps of 2.338-2.350 eV respectively while InP has a direct band gap of 1.4236 eV [26]. The exact band gap determination for GaP is complicated due to the presence of camel's back structure in conduction band minima of X-valley [27]. Further for AlP, there is confusion about the ordering of conduction band minima whether it follows X- $\Gamma$ -L [28] or X-L- $\Gamma$  [29].

Group II-VI semiconductor consists of an IIB metal (e.g. Be, Mg, Cd) combined with the anion from a VIA (e.g O, S, Se, Te) of periodic table. Due to large difference in electron affinity of the constituent elements these compounds are more ionic as compared to III-V compounds [30]. The binary beryllium chalcogenides being

II-VI semiconductors crystallize in zinc blende phase while wurtzite is reported as ground state structure for BeO [31, 32]. These substances have special features of small ratio for ionic radii along with high degree of covalent bonding [30]. Beryllium chalcogenides have indirect band gap with minimum gap along  $\Gamma$ -X symmetry direction [33]. Further the higher value of bulk modulus and larger band gap makes these materials harder and more stable [33]. There are reports about decrease in hardness and increase in the band gap for BeS with increase in the concentration of Te [34]. Further the first principle calculations with TBmBJ approximation have been found to provide an improved description of band structure and optical properties of BeX (X=S, Se, Te) [34].

The Magnesium Chalcogenides due to their wide band gap and low dielectric function are promising candidates for fabricating the optical devices working in ultraviolet region and high temperature electronic devices [35-37]. These materials can crystallize in wurtzite, zinc blende and rock salt structure. There are certain controversies about their ground state structure. The experimentally reported ground state for MgO, MgS and MgSe are cubic rock salt structure, while hexagonal wurtzite phase with space group 186 (P6<sub>3</sub>mc) for MgTe [31]. However recent first principle calculations reported NiAs structure as ground state structure for magnesium telluride [38]. These observations are supported by theoretical prediction of polytypism which is dominated by wurtzite phase [39].

In the last series of our present study is CdX (X=O, S, Se, Te). CdX as II-VI binary compound semiconductor are of increasing interest due to their potential applications in fabrication of optoelectronic, photovoltaic and spintronic devices [40]. Cadmium chalcogenides forming a part of transition metal chalcogenides have also been considered as more suitable material system for photovoltaic (PV) cells as compared to the main stream PV materials like lead perovskites and organic photovoltaic (OPV) [41]. This is due to the greater stability of the Cadmium chalcogenides as the lead perovskites and OPV materials have greater sensitivity to the water and oxygen [42, 43]. Although the Cadmium solar cells are still under development, the first solar cell with CdTe thin films set a new record efficiency of 22.1% [44]. However the high toxicity of Cd restricts the Cadmium chalcogenides as photovoltaic material to the laboratory scale test [41]. Regarding the fundamental properties, CdO is found to be stable in rock salt while the chalcogenides of Cadmium

prefers to crystallize in zinc blende structure under ambient conditions [40]. Further due to the presence of highly localized d orbital in valence shell of Cd, the first principle DFT calculations using local and semi local XC functional fail to predict accurate electronic properties of these materials. For example CdO is reported as a semimetal [45] while experimental results showed an indirect band gap of 0.9 eV for rock salt phase [46]. Additionally, the energetic position of occupied d orbital is wrongly predicted about 3 eV higher than the experimental values [47, 48]. In order to find a solution to these problems PriyaGopalet. al. tried the ACBN0 [49] functional and found that although ACBN0 improved the results over PBE still some under estimation for cadmium sulphide cadmium selenide and cadmium telluride exist [50]. Further the band gap for CdO had been found to be overcorrected.

## 1.2 Literature survey

In order to solve the problem of overestimation of lattice constants of solids by GGA XC functional given by Perdew et. al. [15, 16], Wu and Cohen [17] introduced a new exchange energy functional. When combine with PBE correlation functional [15, 16] the new XC functional so formed was supposed to improve the results over PBE. In order to test the performance of this newly proposed functional F. Tran et. al. [51] performed the calculations for geometrical parameters of 76 solids along with the binding energy and surface formation energy of h-BN layer to the transition metal surfaces. In addition calculations for molecules had also been performed. Their results showed that for III-V semiconductors including 4d and lighter 5d elements along with their compounds, WC performed better than PBE functional [51]. The WC optimized lattice constants lay in between those calculated with LDA and PBE and were much closer to the experiments[51]. For molecular systems though PBE remained better functional. The results for surface calculations were found to be better by WC in case of lighter elements however LDA produced the better performance for heavier elements. In 2008 Perdew et. al. [18] proposed a new XC functional named PBEsol, for solids and surfaces. This functional has been designed to improve the equilibrium properties of solids. M. Ropo and K. Kokko [52] tested the accuracy of PBEsol by calculating the equilibrium geometrical parameters and bulk modulus of 10 simple metals and 19 transition metals. They showed that lattice constants and bulk modulus calculated by using PBEsol had been in close agreement with those obtained with PBE, AM05 XC functionals.

P.Haas et. al. [53] tested the semi local functionals for the calculations of lattice constants of 60 solids taking the elements from different parts of the periodic table in their test set. The results showed that LDA underestimate the lattice constant with mean error (ME) of - 0.058 Å while PBE overestimate with mean error of 0.051 Å [53]. The newly proposed semi local functionals like WC, PBEsol improved the results for lattice constant over LDA and PBE by reducing mean error to 0.01 Å and -0.05 Å respectively. Although these new functionals provided better results on an average but for different classes of materials, different functional performs better [53]. They concluded that no functional reproduced the experimental result with minimum error for all types of the materials in their study. Further interatomic pair potential calculations for alkali metals and IB group metal using the eight different XC functional also lead to the conclusion that different functionals have variable performance with change in the material [54]. Even for same material but with different crystal structure XC functionals performed differently. Recently a new exchange correlation functional SCAN (Strongly Constrained and Appropriately Normalised) is proposed by Sun et al. [19] which has been satisfying all the 17 applicable constraints to a meta GGA as compared to standard GGA which satisfy only 11 constraint. In selecting the correct ground state structure, SCAN was found to reduce the error from 12% to 3% when compared with GGA including as studied by Y. Zhang et.al. [31]. Including SCAN in testing set of functional. Zhang et. al. [54] found that this newly developed functional outperforms all the six XC functionals included in their study in calculating the cohesive properties. However the mean absolute relative error in estimating the lattice constant for semiconductors is 0.5% slightly greater than that produced by PBEsol 0.4% [54], so evaluation of scan functional still needed to be tested for this class of the materials. A similar type of the study is performed by Tran et. al. [55], in calculating the cohesive properties of 44 strongly and 5 weakly bound solids using different functionals, lying on first four rungs of Jacob's ladder. From there study the authors concluded that although SCAN provided a better agreement with the experimental the lattice constants yet it fails to improve the band gap as compared to GGA. In fact no meta GGA included in their study had found any improvement in the band gap [55].

In Kohn Sham scheme based density functional theory the term band gap refers to the energy difference between the Conduction Band Maximum (CBM) and Valence

Band Maximum (VBM). The experimental band gap on the other hand is defined as the difference between ionization potential and electron affinity. Theoretically the fundamental band gap differs from the Kohn Sham band gap by the term, called as, derivative discontinuity ( $\Delta_{xc}$ ) of exchange correlation functional [56, 57]. Here  $\Delta_{xc}$  depends upon variation in exchange correlation potential with the change in number of electrons (N). For the standard density functional i.e. LDA and GGA, due to smooth dependence upon N,  $\Delta_{xc} = 0$ . Although, for exact exchange correlation functional  $\Delta_{xc} = 0$  has been found to have a finite value. As a consequence LDA and GGA underestimate band gap [58]. Thus alternative methods have to be used in order to get the accurate band gap prediction. Hybrid functionals [59] and GW [60] approximation are known for better description of the band structures in solids [61, 62]. But due to their high computational cost these approximations are less applicable for the large systems. LDA+U [63] scheme provides better band gaps at less computational cost but are applicable to localised electrons (i.e. 3d or 4f) only. Thus a method is needed which can reproduce the experimental band gap in an efficient way but at the lower computational cost. In order to solve this problem Tran and Blaha recently proposed an exchange potential (known as TBmBJ) [20] which leads to an improvement over LDA and GGA results for various classes of the materials. Efforts for further improvement in TBmBJ potential by Kolleret. al. proposed new parameterization to the existing mBJ potential [64].

Since the development of TBmBJ approximation, a number of tests have been performed for accuracy in reproducing the experimental band gaps of the solids. For example Kim et. al. [65] calculated band structure and effective masses of III-V semiconductors using GW, hybrid and mBJ approximation. For mBJ calculations they optimise the parameter 'c' for each material in order to fit the experimental band gap. They observed that mBJ exchange potential in association with LDA correlation energy provide the band gap description with accuracy in the scale of more accurate GW and hybrid approximations and at a lower computational cost. However the effective masses had been found to be overestimated by 20 to 30 % with mBJ [65].

David Koller [66] used mBJ approximation for predicting the band gaps of non-magnetic transition metal oxides and sulphide, ferro and antiferromagnetic materials. They showed that TBmBJ approximation can describe accurately not only the band structure but the other properties like magnetic moment and electron density also [66].

The authors also found that there exists certain examples (like  $\text{EuO}, \text{Cu}_2\text{O}$ ) where TBmBj potential have been found to be not accurate [66]. On the basis of their observations the authors suggested for further improvement in the optimisation of parameters 'c' appearing in expression for mBJ exchange potential [66].

D. Singh's [67] testing of TBmBJ potential for electronic and magnetic properties of condensed system showed an improved description for semiconductors and insulators as compared to the standard GGA. However the position of 3d states in zinc oxide and 4f state in case of  $\text{La}_2\text{O}_3$  found to be different from those obtained with LDA+U approximation which is considered to be accurate method for the description for localized orbital [67]. In addition ferromagnetic properties of Gd had also found to be seriously degraded with mBJ potential [67]. In order to correct the binding energy for localised states like d/ f states H. jiang [68] proposed a perturbation approach which combines the Hubbard U potential with the TBmBJ potential. This new approach had been found to improve the energetic position of semi core states as compared to the original mBJ approximation but at the cost of a slight overestimation of band gaps [68]. Further TBmBJ approximation has been successfully applied for predicting the electronic structure of transparent oxide by H. Dixitet. al. [69]. Later on Tran and Blaha [70] compared the results for band gaps of 76 solids using various functional with special attention to the potential HLE16 [71]. According to their study mBj potential is the most accurate method as compared to the all other semi local potentials included in their study [70]. Further the dependence on the kinetic energy density makes the mBj potential more appropriate as compared to other semi local potentials.

### 1.3 Motivation of study

As already discussed in the last sections, the wide band gap values of III-V and II-VI semiconducting materials makes them potentially applicable in modern technologies like optoelectronic devices working in wide range of electromagnetic spectrum, high temperature/power electronics and the devices working efficiently in the harsh environmental conditions. Further alloying other elements in the host material can alter their properties which lead to the modification in performance of the existing devices. All these things make it necessary to understand basic optoelectronic properties of these materials. Regarding the methodology to be adopted for studying these materials, we are attracted by DFT based computational methods which are growing up as the strong tool for predicting the ground state properties of solid state

materials in Modern era of the fast and accurate computing system. In DFT, since the accuracy in results depends primarily upon the exchange correlation functional. Therefore, it is pivotal to select proper functional. From an intensive literature survey we came to a conclusion that there exist no universal functional which is optimal for all classes of the material and even for all types of the properties of a given material. One has to make a testing of a number of functionals for calculating the desired properties of a given class of materials. With all these things in mind, we started our work with the objectives as mentioned in the following section

## 1.4 Research objectives and organization of thesis

The present thesis work has been performed with following research objectives:

- (i) First of all, theoretical calculations of electronic like electronic band structure, DOS, Fermi energy, band gap, etc of properties of group III-V (AX; A=Al, B, Ga, In; X= N, P) and II-VI (BY ; B= Be, Mg, Cd ; Y= O, S, Se, Te) wide band semi-conducting materials were carried out.
- (ii) Further, the optical properties both linear and non-linear of these semi-conducting materials were investigated.
- (iii) Finally, theoretical calculations under extreme conditions (like high pressure and high temperature) were also carried out in some cases wherever it is necessary.

In order to accomplish the first objective i.e. the calculation of the ground state properties of the materials under study we used five different XC functional in calculating lattice constant and bulk modulus while for predicting the band gap, we performed the calculations using modified back Johnson potential as suggested by Tran and Blaha in its original and improved form. Next, using the electronic band structure so obtained we further went for the calculation of the various optical properties of the materials under study. Among them the linear optical properties calculated are dielectric functions, the frequency dispersion curve for real and imaginary part of the dielectric functions, refractive index and energy loss.

All these calculations were performed using the full potential linearized augmented plane wave method as implemented in win2k code although some studies were also performed using TBLMTO (Tight Binding Linear Muffin Tin Orbital) code.

Further, due to non availability of the nonlinear optical properties in win2k code, we used the ELK code which is also based upon full potential linearized augmented plane wave method. Among the materials studied, the second order susceptibility of some of the materials having no inversion symmetry have also been calculated. Further some high pressure phases i.e. rock salt phases of three nitride materials were also studied. The thesis is organised in six chapters the first chapter deals with the general introduction to the problem in hand along with the literature survey and Research objectives. The second chapter deals with a brief review of the methodologies used in the present study. In the third chapter we presented the results calculated for the lattice constant of all the studied material using the five different functional along with the comparison with some recently reported results using the same functionals as well as some other functionals also. In the fourth chapter the calculated band gaps using the standard density functional and modified Becke Johnson potential in its original and improved form are presented. All the electronic and optical properties were calculated using the optimised lattice constant. In this chapter we also report the band structure and density of state plots for the various materials. Chapter fifth includes the calculated values for the optical properties both linear as well as non linear of the materials under study. At last in the chapter sixth the concluding remarks and future prospective of the present study have been discussed.

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