Review on first principle study for progression to investigate the properties of semiconductor compounds

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Abstract

Over the last decade, the first principle study, has achieved a great importance in the field of quantum chemistry, solid state physics and material science. This study is about to investigate the different prosperities of many-body electronic systems and it is a quantum mechanical simulation approach. Eventually, this approach has a tool to predict some new materials and their properties computationally. This method can save the use of chemical methods, which can be harmful to the environment. In this review article, the research field of first principle techniques has been explored for some important semiconductor materials.

Keywords: - First principle study, Structural properties, electronic properties, semiconductor material

Brief overview of density functional theory:-

Over the last two decades, the first principle study became popular for determining different properties of complex systems (i.e. many body electron system). The study can apply in the different field of science like solid state physics, quantum chemistry, and material science. In material science, it can have a good impact for determining the different important parameters of different semiconductor materials, liquid crystals, polymers, radioactive materials, insulating materials etc. The number of research publications can predict the success story of any research field. Fig. 1 is showing here the year-wise increasing trend of the first principle study. Research trend of the first principle applications in quantum chemistry for complex systems began popular only after 1990. This approach became more popular after getting the prestigious Nobel Prize in 1998. It was Walter kohn and John A Pople who received the Nobel Prize who developed some new formalism for understanding the atomic bonds in molecule. This is quite unexpected that this approach originated from the research article of Hohenberg, Kohn, and Sham earlier. Along with this, the combined calculation of Density Function theory and molecular dynamics provided a well defined structured way to observe the structures and the reactions between atoms in molecules for extended complex systems [1].

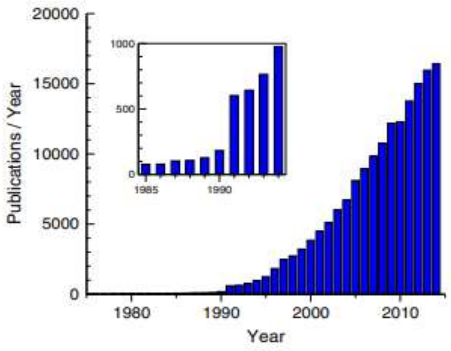

Figure 1 Year wise (1975–2014) publication growth on topics density functional theory.
(From Mavropoulos, 2015).

Not only in quantum chemistry, but first principle study has become useful for calculations in solid state physics also after 1970s. Particularly, LDA achieved more popularity among all quantum mechanical simulation approach as it gives always the adequate determinations (approximations) with experimental one. After introducing the exchange-correlation interaction approximation first principle study became useful in quantum chemistry after 1990s. A model was developed to understand the interactions of electrons in a complex system. Now days, DFT has grown such a way that it leads among many field, especially it gives impact on material science. However, still researchers have faced difficulties to solve the complex systems, band-gap in semiconductor compounds and strong dispersion systems. So, DFT is still a developing field in research [2]. Now, the present review article is focused on the study of the different first principle approach to determine the different properties such as structural properties, elastic properties as well as electronic properties of different semiconductor compounds like different nitrides, chalcogenides compounds etc.

Metal nitrides:-

In recent timings, the group-III nitrides and their alloys have attracted the interests of the researchers towards the analytical research about materials. As, the metal nitrides semiconductor materials such as AlN, GaN, and InN gives wide range band-gap, so those materials are technologically very important. Each metal-nitride semiconductors are having some optoelectronic applications. Those are having short-wavelength, which vary additionally for high values of temperature, frequency and power of electronic devices. Blue light-emitting diodes with high efficiency, LEDs, square measure, laser diodes are some commercially available devices which is an application of those materials.

Ferhat et al. [4] have studied, BSb in B3 form, and compared their results with the results obtained for BN, BP, and BAs. The calculations were done using plane-wave enlargement among the native density approximation. They have computed the lattice constant, bulk modulus [3]. The ab-initio computation of the electronic and structural assets of B3 in $Al_xGa_{1-x}N$ and $Al_xIn_{1-x}N$ alloys were completed by Kanoun et al. [4]. In this study, all-electron FP-LAPW inside DFT was used. The resulted obtained showed that lattice constant coefficient of elasticity B varies linearly with x.

The experimental investigation for InN and alloy InGaN has been done by Walukiewicz et al. [5] .They have used thin film technique for the investigation. The Optical absorption, photo-modulated, reflectivity, photoluminescence, and soft x-ray chemical analysis revealed that the space temperature band gap of InN is 0.67 ± 0.05 eV.

The trend of band gap in alloy AlxGa1-xN and InxGa1-xN has been examined by Gonzalez et al. [6] using first principle approach. They have used FP-LAPW for calculation the parameters. For Nitrides the super-cell was formed for wurzite structure. The exchange and correlation function of PBE96 and EV93 respectively have been employed by them. The predicted band gap was direct in nature. Beloufa et al. [7] reports the quantum mechanical simulation with the ab-initio approach to calculate the different electronic and therefore the structural properties of Aluminium Nitride, Gallium Nitride, Indium Nitride, Aluminium Gallium Nitride and Indium Gallium Nitride in several unit cell structures. The study has done with the method of full potential linear muffin-tin orbital (FP-LMTO), which a computational approach and plane-wave basis has used for coding. The generalized gradient approximation (GGA) took into account for energy calculation. The obtained results of different properties of the above mentioned compounds has been taken for two different structures that is B3 and B4 phases and compared to the theoretical works and with other experimental determinations. They have additionally applied this process methodology to Aluminium Gallium Nitride and Indium Gallium Nitride alloys to envision its fungibility to calculate the structural and electronic properties of their binary compounds. For the alloy BxIn1-xN the structural and electronic properties are determined by Abdiche et al. [8] in the zinc blende phase. The technique used by them was based on FP-LAPW.

Firstly, they have computed the structural properties like lattice parameter, bulk modulus etc. then, the electronic investigations was done like band gap and densities of state. They have concluded that for the x=0.75, the alloy is semiconductor with large band gap and it can be used as an excellent material in the field of optoelectronic.

Some metal chalcogenides:

Barium chalcogenides:-

The structural, electronic and high pressure properties of barium chalcogenides has been calculated by A.Bouhemadou et al. [9] For the energy value calculations the exchange correlation potential has used, which is an approach of the local density approximation and generalised gradient approximation. The determined lattice constant and bulk modulus agrees with the evaluated experimental data and other computational values of the parameters. They have reported that the calculated band gaps in their respective research work, using LDA and GGA approximations are in excellent comparison with other simulation techniques data, but slightly different with experimental data. The electronic properties of barium chalcogenides were systematically observed by G.Q. Lin et al. [10] using DF theory computations, based on both generalised gradient approximation (GGA) and local density approximation (LDA) using CASTEP coding. They have reported that the compounds are containing oxygen atoms have always shows some different behaviour with electronic properties, whereas, the compounds without oxygen atoms don't show. E. Tuncel et-al. [11] performed the first principle approach based on norm-conserving pseudo potential and DF computational theory using SIESTA coding. The programming had been done within the LDA approximation to determine the several properties like structural, thermal, elastic and lattice dynamical properties of Barium chalcogenides in B1 and B2 structure. They have observed the phenomena of phase transition from B1to B2 structure, and elastic properties. The structural and elastic properties of barium chalcogenides under high pressure have been investigated by Balwant S Arya et al. [12] using two body inter-atomic potential approaches with modified ionic charge. The equation of states in NaCl type to CsCl type structural phases for BaX(X=S,Se and Te) has been depicted They concluded that the calculated values of phase transition pressure, equilibrium lattice constant and cohesive energies of these compounds are in excellent agreement with the available experimental data and since the change in cohesive energy from NaCl structure to CsCl structure is positive quantity. Purvee Bhardwaj et al. [13] has determined the change in structure under a conditional high-pressure of several Barium chalcogenides using a three-body interaction potential MTBIP coding, It has used after changing the incorporating covalency effects. They have considered a zero-point energy effect. Zero point energy is the minimum energy, at which compound may possess, and generally, the ground-state energy of the compound may defined as zero point energy. Using the values of model parameters they have obtained the values for phase transition pressures and associated volume collapses from TBIP which shows an excellent coordination with exist experimental data. As the radii ratio of cation to anion changes the conditional phase transition pressure for B1 and B2 structure changes inversely. A. Benamrani et al. [14] have performed ab-initio calculations with the pseudo-potential plane wave approach. The local density approximation (LDA) and the generalized gradient approximation (GGA), which is a quantum mechanical simulation approach was used. In both NaCl and CsCl structures using ABINIT coding has used to determine the different properties of BaX (X = S, Se and Te). The elastic, vibrational properties and lattice dynamics are calculated with the LDA and the density functional perturbation theory. By changing the volume of unit cell the change in pressure estimated and with this the structural, vibrational and lattice dynamics has been studied. They have reported the determined value of elastic and vibrational properties and lattice dynamics using perturbation approach of DF theory and the calculated elastic constants was having well and good agreement with the other calculated values using LDA–FP-LAPW.

Strontium chalcogenides:-

Strontium chalcogenides are important as those materials are having a high transitional pressure, at which the structure of the crystal unit cell transforms from one phase to another phase. Primarily those materials are having NaCl structures but after transformation with some conditional high pressure it transit from NaCl to CsCl structure. Strontium chalcogenides SrX (X = O, S, Se, and Te) are technologically important as those materials are having broad technological application in television picture tube glass, catalysis, microelectronics, luminescent devices, radiation dosimetry, fast high resolution optically stimulated luminescent devices, and infrared sensitive device. Many theoretical investigations to investigate the structural properties of those technologically important compounds had been done by many researchers.

Varshney et al. [15] discussed about the structural parameters of the strontium chalcogenides compounds. They have chosen four compounds specifically as their sample that is SrO, SrS, SrSe, SrTe. They have discussed two parameters in structural properties that are lattice constant (a_0) and bulk modulus (B_0). Also they have observed a conditional phase transition from one stable structure to another, for those particular compounds. Like Manal M. Abdus Salam [16] also have reported in his research paper that Strontium chalcogenides transit always from B1 phase to B2 phase under a conditional high pressure. But he has taken only but he has taken only the case for SrO, SrSe and SrS. To calculate the structural phase transition he has calculated Gibbs free energy first from the equation, G = U + PV – TS and also put T=0K. So the equation will be automatically change into G= U + PV = H (Enthalpy). Then they have ploted the graph between the enthalpy and pressure and deducted the value of transitional pressure (P_T).

Alkali hydrides:-

N Novakovic et al. [17] used the Full potential lineralized augmented plane wave method to calculate the electronic structure, optimization of volume, bulk modulus, elastic constant and frequencies of the transversal optical vibration in the LiH, KH, RbH and CsH compounds. Along with this they have also illustrated several selected experimental results, not only that but also talked about different theoretical approaches respectively used in purpose of various alkali hydride properties. Sinem Erden Gulebaglan et al. [18] used the first principle calculations to determine the electronic, optical, elastic as well as thermodynamic and lattice dynamical properties of the compound RbH. It has the B1 structure. Plane wave pseudo potential method has been used in this work to determine the band gap and lattice constant which are the ground state properties. Moreover some other properties like internal energy, specific heat, Helmholtz free energy and entropy have been followed in this work. Suman Banger et al. [19] calculated the structural stability and elastic constants of alkali hydrides (LiH, KH, NaH) by using the FP-LAPW method which is first principle approach. To explain the exchange correlation functional the GGA has been used. The result of their work also compared with other observational data.

Some other important compounds:-

Munjal et al. [20] have investigated the transitional pressure from B1 structure to B2 structure and cohesive energy of MgO by first principle method. The calculation has been donewith the density functional theory (DFT) approach. Linear combination of atomic orbitals (LCAO) method has been utilized using CRYSTAL06 code. They have performed the calculations based on the generalized gradient approximation (GGA) proposed by Perdew-Burke- Ernzerhof (PBE) and Becke's scheme to treat the correlation and exchange effects respectively. Their study reveals that energy states of B1 phase is below the B2 phase, which indicates that the B1 phase is more stable than B2 phase. In their calculations, they have considered zero temperature at which the thermodynamically stable phase is that one with lowest enthalpy, H = E + PV at a given pressure. The transition from one phase to another phase appears, after the intersection of enthalpy of two

different systems. Those two different systems are the states having lower energy and the states are having higher energy. After the point of coincident, the enthalpy value of B2 state becomes low than B1 state. Hence, they concluded that NaCl state (i.e.B1 state) is having more stability at the low pressure whereas the same can be followed for CsCl (i.e. B2 state) state at very high pressure.

Brik [21] has used the ab-initio approach using the CASTEP code to determine properties of $CuXS_2$ for different X of group 3. For energy correlation the Materials Studio package has utilized, Sellmeyer's approximations have been used for finding the index of refraction.

Conclusion:-

First principle studies are very useful and approachable to the scientific community for doing the research in the field of quantum chemistry and material science. This is also known as ab-initio method and also a density functional computational method. The quantum mechanical simulation approach has been performed. The technologically important different materials like metal nitrides, metal chalcogenides and some other compounds has explored in this article. Different approaches like FP-LAPW, LCAO, CASTEP etc. has been explored for doing the computational study to determine the different properties. Those properties are important to know for the further technological development using those materials. Using those approaches the use chemical analysis can be reduce to determine the different properties of binary compounds and their alloys can predict their applications easily.

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