The Optoelectronic Property Analysis of P doped SrGeN₂: A First Principle Calculation for Solar Cell Compound

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Abstract. The first principle investigation of P doped SrGeN₂ - a wideband semiconductor is undertaken to prove the beneficial usage of the compound in a particular optoelectronic application field. Wideband semiconductor is the semiconductor compound that contains a larger energy gap difference in comparison to the traditional semiconductors. But to utilize the compound in the form of a particular application like solar cell, bandgap engineering for the compound is followed to reduce the bandgap as per required value range. For this purpose, doping feature is introduced in the bandgap engineering procedure and can be done at a particular site to gain the desired energy gap. Thus the investigation of the properties to learn about the optical, electronic and structural features of the P doped SrGeN₂ compound is done using the Tran Blaha modified Becke Johnson (TB-mBJ) exchange correlation. The exchange correlation is rooted in the framework of DFT based on the first principle-linear augmented plane wave methodology. This paper deals with varied property analysis schemes like structural, optical and electronic behaviour deployed in DFT framework stating the value of absorption curve and dielectric tensor which is analysed for the optical property study with integrated absorption curve value being 33.681 and static dielectric tensor value ε(ω) being 4.28 in case of P doped SrGeN₂ gained through mBJ potential.

1. Introduction

XYZ₂ (X=Sr, Mg, Ca, Be; Y=Ge; Z=N) sample is introduced as group II-A, IV & V type of chalcopyrite material with a noticeable wideband. The application of wideband compounds is observed to find its utility in optoelectronic devices or electronic devices [1]. Semiconductors providing tuneable band gap
is included as II-IV-V₂ ternary compounds. II-IV-N₂ compounds are tetrahedrally bonded with the group-III nitrides derived from wurtzite structures gaining attention in material field. In the work by Tang and Gao, phonon calculations for Cd-IV-N₂ and Zn-IV-N₂ have been done in order to check the dynamical stabilities of lattice [2]. Also the DFT calculations using the ABINIT package has been done. ZnGeN₂ has proved to be an interesting compound with its lattice nearly matching to GaN (working as analogue of GaN) and bandgap offered to be 3.6 eV [3-4]. This compound is assumed to have tunable bandgap useful for optoelectronic active layer ranged 2.6 -3.4 eV [5]. Using AlN templates and GaN buffers, ZnGeN₂ thin films were produced by MBE. The essential step for optoelectronic devices has been done by the significant development of hybrid ZnGeN₂-GaN [6]. Another work by Punya and Lambrecht [7] has shown the performance of ZnGe0.5Sn0.5N₂ and CdGeN₂ by first principle investigation. Study of various p-type dopants like Ga, Al, Cu, C, Li, Na, and K in ZnGeN₂ has been done computationally using the first principle investigation [8]. Orthorhombic in nature with wideband feature exists in MgSiN₂ and MgGeN₂ compounds whose structural and other properties are examined [9]. Through the DFT calculations, the band alignment of some compounds like MgGeN₂ has been studied. The pseudo-potential methodology was adopted to calculate the energy band gap for every compound [10]. The benefit of having a wide-bandgap compound is that it offers an option to alter bandgap according to application’s suitability along with high thermal conductivity, stable high temperature electrical performance, large field strength of breakdown etc. [11]. Thus we can say that these wide band compounds are important in electronic devices of today such as p-n junctions, transparent contacts, thin film transistors etc. with the features of good optical transparency of a higher range, balanced carrier concentration and electrical conductivity which can be tuned [12]. History has seen investigation of oxide based wide-bandgap compounds due to their antithetical high transparency and conductivity properties.

The most abundant form of energy i.e. clean and safe both is the solar form of energy which aids in empowering the economic growth of the society. The state of art of devices is analysed with a recent 5-year progress graph of photovoltaic (PV) technologies which helps in marking the future growth of PV cells [13]. IBSC (Intermediate band solar cells) provides an improved efficiency in energy conversion technique in case of solar cells with single gap. To provide improved energy conversion efficiency in IBSCs techniques like quantum dot (QD) nanostructures and use of highly mismatched semiconductor alloys is done [14]. The ideology behind solar cells is to provide a powerful solution for power saving display systems, power generating windows, wearable electronic devices, self-powered flexible, building integrated photovoltaics space craft and satellite applications, charging of e-vehicles and solar lighting etc. Photovoltaic performance is affected by various factors of SCs e.g. solar cell architectures, operational and thermal stability challenges, photovoltaic materials, recombination losses, photo-electrode materials, thermal and chemical treatments, trap defects, optical irradiation and hole transport materials [15].

2. Computational Details

The density functional theory framework was implemented within the necessary set of boundary conditions as guided in Wien2k software. Calculations based on Quantum mechanics aid in determining the properties of a material along with giving a perspective of the new properties that can be explored. Different models based on theoretical approach are followed to study the behaviour of electrons and atoms of a material [16]. For the total energy calculation, GGA functionals are known to be very common but provide a bandgap which is underestimated than the experimental value [17]. An enhanced version of Becke Johnson potential [18] as an exchange constitute the Tran-Blaha modified Becke Johnson (mBJ) [19] approach and is accompanied by LDA [20] as correlation that regenerates almost accurate KS potential [21].

3. Result and Discussion

3.1 Structural Details

The structure of SrGeN₂ is constructed in the XCrysten tool of Wien2k and the structure formed is tetragonal with space group being I-42d viz. numbered 122. When doped with P it offers a space group of 81-P4 in the newly constructed structure. The structure contains three atoms namely: Sr, Ge and N.
which are combined together tetrahedrally. The total number of atoms formed in this cell structure are 22, with 8 Sr atoms, 6 Ge atoms, 7 N atoms and one P with their respective positions. The optimized lattice parameters involve $\alpha=5.1897$ Å, $\beta=5.1897$ Å & $\gamma=8.8220$ Å located at Wyckoff positions for elements as Sr (0,0.5,0.75), Ge (0,0.5,0), N (0.066, 0.816, 0.812) & P (0.066, 0.816,0.3125). To understand the stability of bulk structure we calculate the formation energy which is valued to be -31.83 eV.

Figure 1. Structural image of (a) SrGeN$_2$ and (b) P doped SrGeN$_2$ along with its coordinate axis.

3.2 Electronic Details

The electronic details depict band structure and density of states plot for the compound under analysis. The band structure refers to the plot between the k points (Z, $\Gamma$, X, P, N, $\Gamma$) and energy in eV. The band structure analysis reveals formation of indirect bandgap in SrGeN$_2$ observed from the bottom of conduction band and top most of the valence band [22]. The optical band energy of the bulk compound and doped SrGeN$_2$ is calculated to be 2.12 eV and 3.82 eV; 1.70 eV and 2.71 eV by PBE and TB-mBJ exchange correlation respectively. The band structure for TB-mBJ calculation is presented in figure 2. (a), (b), (c). In this direct bandgap can be seen between the $\Gamma$-$\Gamma$ bands of conduction and valence bands. The density of states plot is used to investigate the electronic properties of the compound as shown in figure 2. (d), (e), (f). Density of plots along with partial density of states are explored in this property. Within the semiconductors, determination of concentration of carrier and distribution of the energy of these is known as density of states [23]. The carrier’s free motion is restricted to zero, one or two spatial
Figure. 3. (a, b, c) Band structure in brillouin zone; (d, e, f) Density of States and partial density of states for bulk SrGeN₂, PBE and mBJ of P doped SrGeN₂.

dimensions. Electronically depicting the meaning of density of states stand out to be that the number of electronic states per unit energy per unit volume of the crystal in a band. The significant contributions in the partial density of states can be observed as 5s² in Sr, 4p² in Ge and 2p³ in N. In the case of doping of P in SrGeN₂, additional contribution of P is shown by the 3p shells.

3.3 Optical Details

The optical details include dielectric tensor plot in respect to both imaginary component and real component, absorption coefficient curve, reflectivity and refractivity. The dielectric feature of the sample includes real part of the tensor and imaginary part of the tensor. It also determines the polarization that is parallel and perpendicular to the sample surface [24]. If a band structure is known once then with the help of it dielectric constant’s imaginary part can be calculated. Due to these we can determine the band structure’s accuracy [25]. The imaginary part of dielectric tensor helps in knowing the inter band transitions that take place in the electronic band structure. The real part of dielectric tensor (parallel) and imaginary part of dielectric tensor (perpendicular) determines the material’s dielectric response with respect to an external electric field. Real part of dielectric tensor is measured as 3.67, 5.87 and 4.28 for bulk SrGeN₂, PBE and mBJ exchange correlation respectively. These two parameters are shown in figure 3 (a) and figure 3 (b). Absorption curve for both the cases is shown in fig. 4 (a) depicting the penetration level of light into a material. The low value of absorption coefficient depicts

Figure 3. (a) Real dielectric tensor; (b) Imaginary dielectric tensor for bulk SrGeN₂ and both PBE & mBJ of P doped SrGeN₂ compound.
Figure 4. (a) Absorption Spectra (b) Reflectivity spectra and (c) refractivity for bulk SrGeN2 and both PBE & mBJ of P doped SrGeN2 compound

poor absorption of light on the contrary, higher value of absorption coefficient absorb photons readily exciting electrons to the conduction band. The dependency of absorption coefficient value is on material type and wavelength of light absorbed. The integrated absorption coefficient for Bulk, PBE and mBJ are calculated to be 10.076, 85.584 and 33.681 respectively. The reflectivity spectra offer 9%, 16.9% and 11.75% in the compound of reflectivity and refraction curve offers a refractive index with a value of 1.89, 2.43 and 2.05 for bulk SrGeN2, PBE and mBJ exchange correlation respectively. An optical feature in which the amount of light that is sent back after striking the material is term as reflectivity. Generally, reflection occurs on surface medium and for translucent materials can occur along the volume of material. The refractive index forms an important feature of the material properties along with transparency and spectral dependency of each property [26]. Reflectivity and refraction curve is shown in figure 4(b) & 4(c).

4. Conclusion
The optoelectronic investigation of newly explored Strontium based wideband semiconductor has been undertaken by using PBE-GGA and mBJ potentials in order to decide its field of application. The features like absorption curve, dielectric tensor, reflectivity and refraction has been studied to analyse its optical functionality. Here we get higher value of IAC of doped compound hence this doped compound shows the good optical activity. In the optical plots, we observe isotropic nature for the bulk compound in the initial visible range and for the doped compound we observe near about isotropic nature. The bandgap offered for bulk SrGeN2 compound is 3.82 eV which when doped with P element reduces the bandgap of the system yielding a suitable application as a better solar cell material or find its usage in any other optoelectronic device. So to prove the point stated we doped the compound with P at a particular site and then reported a reduction in bandgap to make a stand in the solar cell domain.

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