



Electronics Structure and Optical Properties of Ag_2BiO_3 , $(\text{Ag}_2)_{0.88}\text{Fe}_{0.12}\text{BiO}_3$: A First Principle Approach



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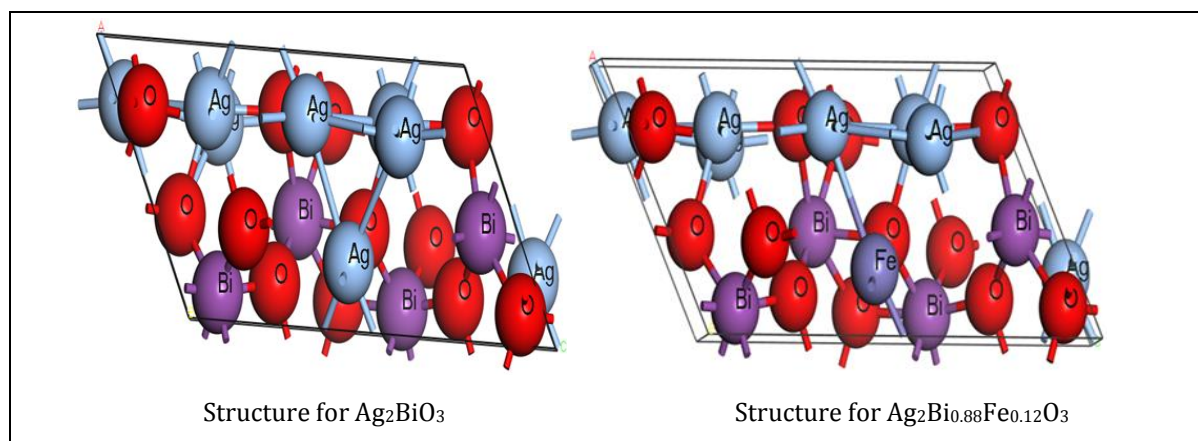
Density of states

Optical properties

ABSTRACT

Electronic band structures, the total density of state, partial density of state and optical properties were investigated using first principle method for Ag_2BiO_3 via Generalized Gradient Approximation (GGA) based on the Perdew–Burke–Ernzerhof (PBE0). The band gap was found to be 0.490 eV which is supported for good semiconductor. The density of state and partial density of state were simulated for evaluating the nature of 5s, 4d for Ag, 6s, 4f, 5d, 6p for Bi and 2s, 2p for oxygen atom for Ag_2BiO_3 orbital travelling from the maximum valance band to minimum conduction band to explain the transition of electron due to hybridization. The optical properties including, absorption, reflection, refractive index, conductivity, dielectric function and loss function were calculated which can account for the superior absorption of the visible light. The key point of this research study was to determine the activity on electronics structure and optical properties for Fe doped by 12%. Regarding the band gap and optical properties, $\text{Ag}_2\text{Bi}_{0.88}\text{Fe}_{0.12}\text{O}_3$ can give more conductivity compared with that than of the Ag_2BiO_3 , showing as a superconductor.

GRAPHICAL ABSTRACT



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Introduction

A common semiconductor is a compound or a solid chemical element which substances face some barrier to the flow of electricity, *i.e.* their properties are almost like conductive or conducting materials [1,2]. Due to the semiconductor technology, over the last 60 years, continuous progress of compounds of group IV, II, VI, and III, V has been made of metals or crystals [3,4]. The electronic structure and optical properties of semiconductors are very important to be evaluated their nature for applications because most of the electronic devices composed by semiconductor regarding electronic structure and optical properties, in semiconductor diode, transistor, and light emitting diodes. Moreover, semiconductors are used to make computers, laptops, and solar cells. Silicon, germanium, and gallium arsenide are used for making semiconductors in initiated time [5,6]. From the arrangement of electrons rotating in different cell paths around the nucleus of a substance's atoms, it is seen that a maximum of eight electrons in cell of atom may be in one orbit. Balance electrons are the electronic components of the cells outside the atom. The outermost cell of an atom can have a maximum of eight electrons, that is, the maximum number of balance electrons is eight. According to the theory of electrons, the nucleus of the nucleus is more or less the number of free or balance electrons located in the farthest cell of the atom. In the case of the transducer, the attraction force of the nucleus is very low, the absorption is too high, and if the semiconductor is between the attractive conductive and non-conductive [7]. This prevents the electrons of the semiconductor material from being transferred from one atom to another. Germanium silicon, carbon, selenium, and acid mixed water are most commonly used as semiconductors while germanium, silicon, semiconductor atomic

structure is a crystalline shape [8]. Besides germanium, silicon, bismuth, iron, and strontium are widely used as semiconductor materials in present time in different advanced electronic device due to their good conductivity [9]. Moreover, the crystal of germanium, silicon, bismuth, iron, strontium and antimony oxide have been established as semiconductor due to their thermal capacity and the forbidden energy gap remains high despite its outer cell having the same balance electrons [10]. Its current conductivity works much higher and at higher temperatures than other semiconductor. Due to these specifications, semiconductor electronics requirements of Ag_2BiO_3 are high.

However, experimentally, Ag_2BiO_3 was shown to be diamagnetic and semiconducting [11,12]. To patch up the inconsistencies concerning the valence state of bismuth in Ag_2BiO_3 they undertook a reinvestigation employing temperature dependent single crystal X-ray diffraction, and neutron powder diffraction, and corroborated the structural findings by measuring the physical properties such as thermal conductivity, magnetism and non-linear optic. Charge ordering is indeed induced by the crystal inversion twin in the Pnn2 phase compared with the Pnna phase. At low temperature phase Pnn, the charge ordering is similar to that of the Pnn2 phase; however, it is more distorted in Pn phase. In addition, the calculation indicated that, the charge ordering is caused in the 6s electron rearrangement [11]. The electronic structure calculations were performed using both the full potential linearized augmented plane wave (FP-LAPW) and the ultrasoft pseudopotential plane wave method, respectively. Within the earlier process, no shape rough calculation is used either for the potential or for the electronic charge density while in the second way, the tightly held core electrons are in the same state as the free atoms, with the pseudopotential in place of the interaction between valence electrons and

atomic cores *via* a nonlocal potential. We make use of the WIEN2K and CASTEP program package within the generalized gradient approximation of Perdew–Burke–Ernzerhof 96 for the exchange–correlation energy.

Experimental

Computational methods

To calculate the band structure, total density of state and partial density of state, using method of GGA with PBE0 was optimized of CASTEP code from material studio [13]. In this condition, the band structure and density of state were calculated using the cut off at 520 eV, and k point at $2 \times 2 \times 3$ with non-conserving pseudopotentials. Then the optical properties were similar way simulated for calculation of refractive index, reflectivity, absorption, conductivity, and loss function. In additionally, the geometric optimization was achieved and the convergence criterion for the force between atoms was 3×10^{-6} eV/Å, the maximum displacement was 1×10^{-3} Å, and the total energy and the maximal stress were 1×10^{-5} eV/atom and 5×10^{-2} GPa, respectively.

Result and discussion

Optimized structure

The lattice parameters value are $a=6.124$ Å, $b=6.359$ Å, $c=9.788$ Å and angels between them as $\alpha=90.000^\circ$ Å, $\beta=91.764^\circ$ Å, $\gamma=90.000^\circ$ Å. The

monoclinic AgSbO_3 crystal and the space group is Hermann Mauguin Pc [14], monoclinic crystal system, point group m, hall $p\bar{2}yc$, and density of 8.24 g/cm^3 are shown in Figure 1a, and the Fe doped optimized structure is accounted in Figure 1a and 1b.

Electronic structure

To determine the electronic band structure of the Ag_2BiO_3 and $\text{Ag}_2\text{Bi}_{0.88}\text{Fe}_{0.12}\text{O}_3$, the Fermi energy level was set as zero. From the Figure 2a and 2b, it was found that the minimum of conduction bands (MCB) were obtained in the Y symmetry point whereas the maximum of valance bands (MVB) were linked also in Y symmetry points. As the both of MCB and MVB are at point Y symmetry, it is called direct band gap and it is calculated by 0.490 eV. As seen in Figure 2a and 2b, both of the upper and lower parts of the conduction band are well dispersive in the near G, Y and A symmetry points than X and D symmetry point. On the other hand, the upper level of the valance band near the Y symmetry point is equally dispersive; however, the lower part is not dispersive. In general, a lower carrier effective mass corresponds to a higher carrier mobility. On the other hand, after Fe doping in Ag_2BiO_3 demonstrates different band structure while the minimum of conduction bands (MCB) were obtained in the Q symmetry point and the maximum of valance bands (MVB) were linked also in Q symmetry points. At the Q symmetry point, the direct band gap was found to be 0.02 eV.

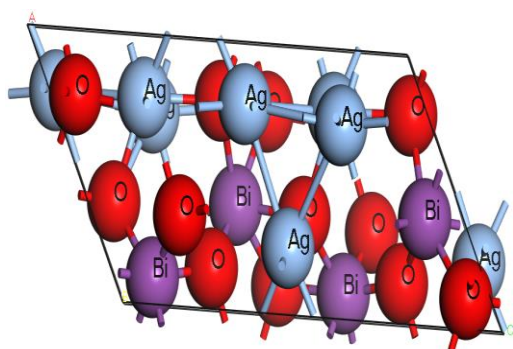


Figure 1a. Structure for Ag_2BiO_3

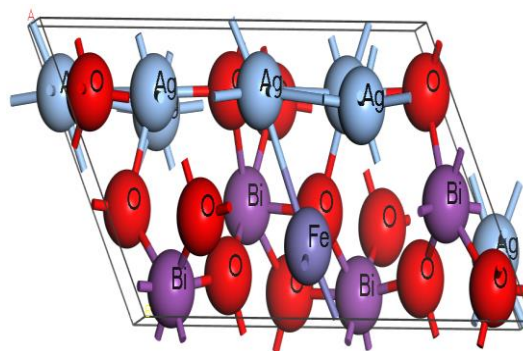


Figure 1b. Structure for $\text{Ag}_2\text{Bi}_{0.88}\text{Fe}_{0.12}\text{O}_3$

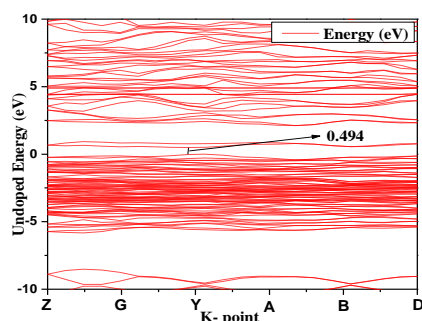


Figure 2a. Electronic structure for undoped

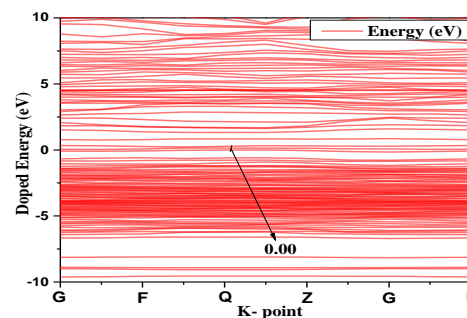


Figure 2b. Electronic structure for doped

Density of state and partial density of state

The density of state indicates the nature of electronic band structures and splitting of orbital. The density of total states (DOS) of Ag, Bi, Fe and O₂ elements for Ag₂BiO₃, and Ag₂Bi_{0.88}Fe_{0.12}O₃ crystals were calculated by PBE0 with GGA. As demonstrated in Figure 3, the valence bands are mainly occupied by 5s, 4d for Ag, 4s, 3d and 4p for Fe and 4s, 3d, 4p for O₂ elements. Meanwhile, above the Fermi level, the conduction bands are composed of Ag in 5s, 4d orbital. As shown in Figure 3, the valence bands just below the Fermi level and the conduction above the Fermi level, it is noted that total density of state for undoped Ag₂BiO₃ is lower than doped Ag₂Bi_{0.88}Fe_{0.12}O₃. It is found that the DOS for s, p, d, and sum for doped is more delocalized than undoped showing in Figures 3a-3f.

Optical properties

Optical reflectivity

As a part of several consecutive theoretical investigations of optical phenomenon, at first, we go through the quantification of optical reflectivity of a crystalline material because it plays a significant role in electronic transition from valance band to conduction band of compounds. The amount of light that is incident on the surface of the semiconductor

materials that can be estimated from the reflectivity data which is related to the absorbance of that material. It is reported in a number of previous investigations that the lower reflectivity indicates the higher UV or visible light absorption. In our investigation, we observed that the reflectivity of Ag₂BiO₃ and Ag₂Bi_{0.88}Fe_{0.12}O₃ commences from around 0.35 and 5.57 respectively at initial frequency and for Ag₂BiO₃, after a successive aggrandizement it reached a falling down of 0.15 at 15 eV and sharply increased at 0.22, sharply falling in about 0.02 corresponding frequency at 23 eV as illustrated in Figure 4. In case of Ag₂Bi_{0.88}Fe_{0.12}O₃, it is changed at same point but smaller than Ag₂BiO₃. It is worth mentioning that, the value of reflectivity saw a dramatic zigzag between 0 to 12 eV; spectacular falling in between 12 and 25 eV and eventually it experienced a linear constant fashion.

Absorption

The polycrystalline polarization method is utilized to calculate the optical absorbance of the Ag₂BiO₃ and Ag₂Bi_{0.88}Fe_{0.12}O₃ material and the method comprises of the electric field vector as an isotropic average over all directions. During the simulation, a small smearing value of 0.1 was applied to attain more distinguishable absorbance peaks.

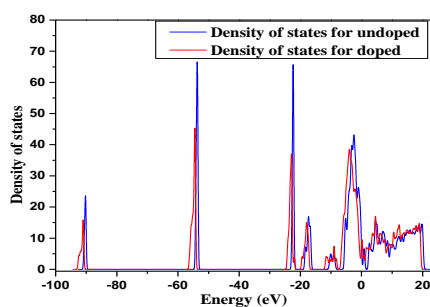


Figure 3a. Comparison of total DOS for doped and undoped

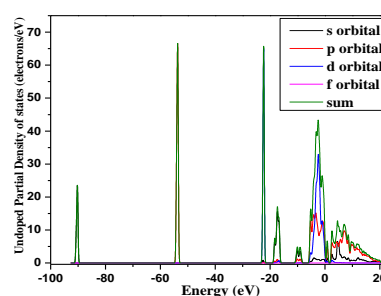


Figure 3b. PDOS for undoped

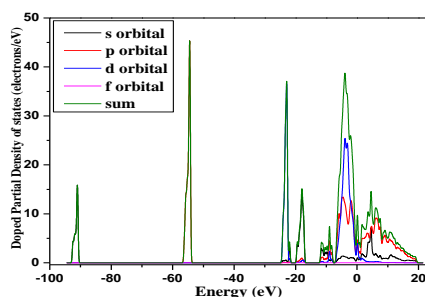


Figure 3c. PDOS for doped

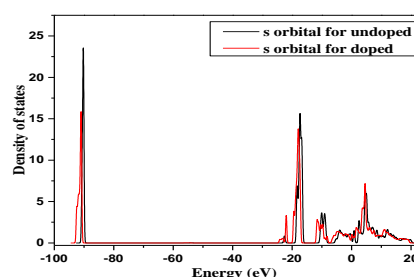


Figure 3d. Comparison the DOS of s for doped and undoped

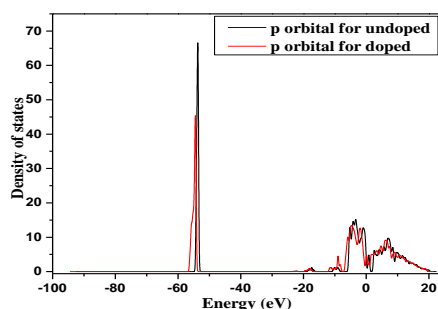


Figure 3e. Comparison the DOS of p for doped and undoped

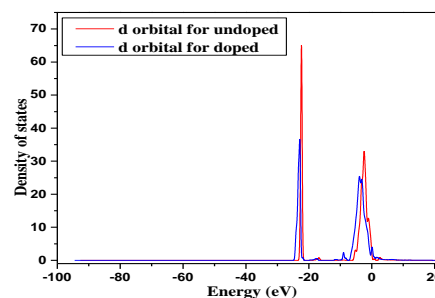
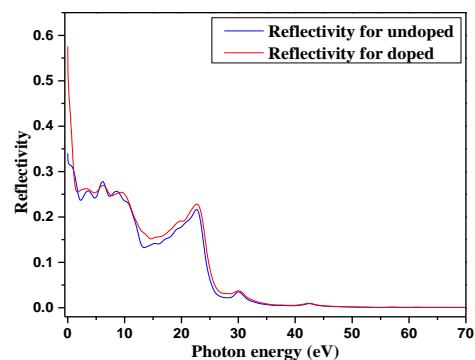
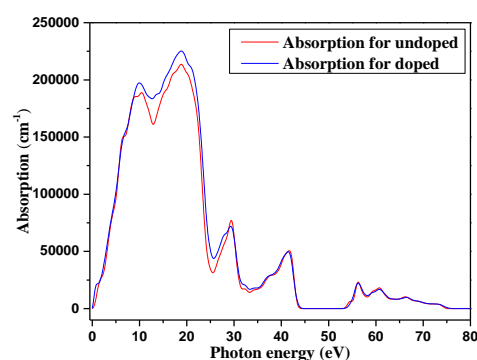
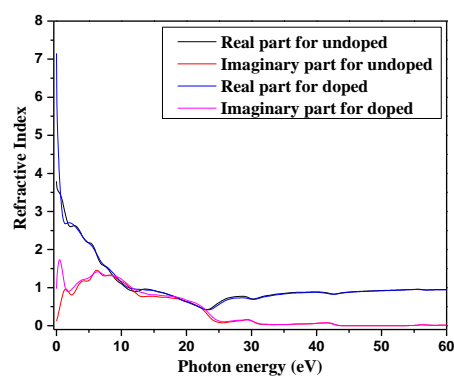


Figure 3f. Comparison the DOS of d for doped and undoped

The obtained absorbance peaks as depicted in Figure 5 is attributed to the photo transition energies from the maximum valance band (MVB) to the minimum conduction band (MCB) under visible light irradiation which indicates that this material can absorb photons of visible range. Both of the Ag_2BiO_3 and $\text{Ag}_2\text{Bi}_{0.88}\text{Fe}_{0.12}\text{O}_3$ revealed change at same point, but $\text{Ag}_2\text{Bi}_{0.88}\text{Fe}_{0.12}\text{O}_3$ was slightly higher than the Ag_2BiO_3 .

Refractive index

The refractive index of a material is an impactful parameter for measuring the photon absorption throughout the process of chemicals degradation from the solutions. Large value of refractive index is associated with the greater denser medium which is reported in a previous investigation. Figure 6 displays the refractive index as a function of photon energy where the real part and the imaginary part for both of the undoped and doped are mentioned, showing an inverse pattern.

Figure 4. Comparison of reflectivity**Figure 5.** Comparison of absorption**Figure 6.** Comparison of refractive index

At initial point of photon energy, the refractive index is higher for real part while the imaginary part is almost closed to zero. The overall decrease of both parts encounters them to each other upto 23 eV photon energy with a value of 0.6 and afterwards they follow a constant pattern with slightly different values of refractive index. It is same for both undoped and doped.

Dielectric function

The dielectric function is very necessary tool to investigate their optical properties which is related with adsorption properties as following equation for solid.

$$\varepsilon = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (1)$$

Where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are denoted the dielectric constant (real part) and the dielectric loss factor (imaginary part) respectively. Dielectric function has a relationship with space

of materials that is physically equivalent to the permittivity or absolute permittivity. The real part of dielectric function represents the energy storage capability in the electric field and the imaginary part represents the energy dissipation capability of the dielectric materials. As can be seen in Figure 7, the imaginary part is less than the real part from 0 eV to 5 eV frequencies; however, from 6 eV to 16 eV the imaginary part is larger than the real part, showing same the real and imaginary part for the doped and undoped.

Figure 7. Comparison of dielectric function

Electrical conductivity

The conductivity of the semiconductor on basis of the energy band and orbitals electrons is linked with the discrete space of electrons in orbit. This is also produced due to the presence of holes and free electrons in the crystal molecules. Figure 8 demonstrates that, the conductivity of doped is slightly bigger than that of the undoped in the both of case.

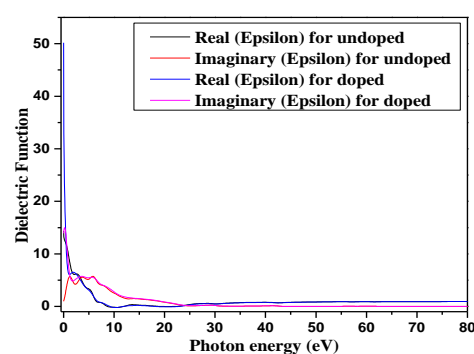


Figure 8. Comparison of conductivity

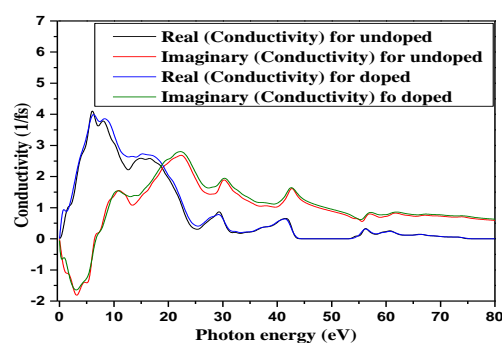
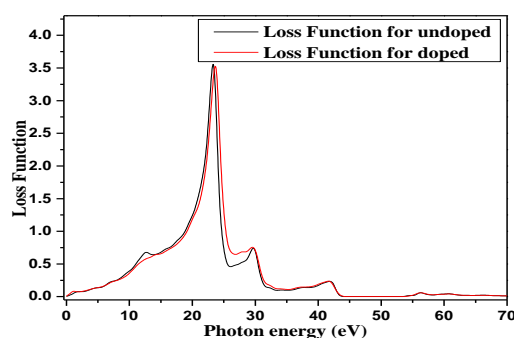


Figure 9. Comparison of loss function



Loss function

There are two regions for electronic energy loss function such as high energy region and low energy region for the optical properties. The first region is the high loss energy region with change of frequency or spectra after the ionization edge which can say the oxidation state of d orbital splitting for metals of center atom in complex compounds, having range the more 20 eV. The other is the low energy loss function, including the energy less than 1, which can provide information about the composition and electronic structure. The energy loss function for optical properties is linked to dielectric constant of the materials within the range of validity of the dielectric theory. As can be seen in Figure 9, the loss function for $(\text{Ag}_2)_{0.88}\text{Fe}_{0.12}\text{BiO}_3$ is about higher compared with that of the undoped.

Conclusion

In our calculation we used the generalized gradient approximation (GGA) on the Perdew–Burke–Ernzerhoff (PBE0) via CASTAP tools within the method to study the electronic structures of Ag_2BiO_3 and $(\text{Ag}_2)_{0.88}\text{Fe}_{0.12}\text{BiO}_3$ crystal. From the electronic structure, the band gap was found 0.494 eV for Ag_2BiO_3 considering as good semiconductor which is almost similar for experimental value 0.510 eV [15] regarding crystal structure in Pnn2. The key point of this study to evaluate Fe doping effect on the electronic structure and optical properties. The band gap was found 0.00 eV after Fe doping by 12% replacing Ag in Ag_2BiO_3 , and the delocalization was also enlarged. On the other hand, a doping activity on Ag_2BiO_3 for the optical properties were estimated, illustrating almost higher than Ag_2BiO_3 . It was also found that, after doping Fe by 12%, the Ag_2BiO_3 almost acted as a superconductor.

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Disclosure statement

No potential conflict of interest was reported by the authors.

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