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First Principles study of Silver Argyrodites-structured compounds A_8BC_6 (A=Ag; B=Si, Ge; C=Te) for Opto-electronic application

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Abstract

The structural and optical properties of a material are studied using Density Functional Theory. By the method of full potential linearized augmented plane wave (FP-LAPW) silver argyrodites Ag_8SiTe_6 and Ag_8GeTe_6 has been investigated. To obtain stable geometry of A_8BC_6 materials, the energy minimization approach is applied. The Generalized Gradient Approximation (GGA) approach is used to optimize the crystal structure of the Argyrodites materials. All these compounds crystalize in a cubic unit cell with lattice constant increasing from 12.13 Å (Si) to 12.28 Å (Ge). The mBJ-functional shows a semiconducting nature Ag_8SiTe_6 for and metallic nature for Ag_8GeTe_6 of these compounds with an indirect band gap lying at the L-X symmetry points with a band gap of 0.24 eV (Si) and 0.0068 eV (Ge) to obtain the optical properties such as refractive index, complex dielectric constant with real and imaginary part of dielectric function, and other optical properties are discussed. Effective mass of electrons is smaller than those of holes resulting in higher carrier mobility for electrons. Due their direct band gap, these Argyrodites materials could be particularly useful in optoelectronic devices.

Keywords: Argyrodites, Optical properties, Effective mass.

1.Introduction

Energy is an essential component of society that contributes significantly to its growth by raising living standards and quality of life. The global energy crisis of today is a major concern for researchers due to the ongoing depletion of energy resources, which is also environmentally unsound. Our primary energy needs are met by fossil fuels, which are neither renewable nor abundant. They will be consumed within the next 50 years, according to some estimates [1]. The scientific community has been compelled to look for more environmentally friendly and sustainable options as a result of the rapid rise in energy demand. The right choice seems to be energy from the sun and waste heat. Solar and thermal energy can be extracted from argyrodites materials. Additionally, thermoelectric energy converters are very important because they can make use of the waste heat that is produced in factories, power plants, and heat engines [2, 3].In the literature on solid state sciences, a series of simple yet fairly efficient empirical models fully or partly based on the ionic radii was reported for predicting the cell parameters of scientifically and technologically important families of cubic crystalline materials such as perovskites ABX_3 [4, 5], defect halide perovskites A_2BX_6 [6,7], pyrochlores $A_2B_2X_7$ [8, 9], and spinel's AB_2X_4 [10, 11].The name "argyrodites" was first given to Ag_8GeS_6, a mineral in which the element Ge was first discovered. Subsequently, a series of synthetic compounds were reported with preparations made by substituting Ge for main groups III, IV and V other elements, partially substituting S for chalcogens or other halogens, or substitute Ag for Cu has been detected [12, 13]. The band structure and optical properties of the recently synthesized compounds Ag_8MX_6 (M = Si, Ge, Sn, X = S, Se, Te) have not been investigated enough. Studies of the crystal growth, crystallography and phase diagrams of Ag_8MX_6 and some results on the electric, photoelectric, and optical properties of argyrodites and canfieldite have been reported. Allots members of the argyrodites, a previously unknown of tetrahedrally close-packed structures families, have been synthesized and described using x-ray technologies. Their generally represented by formula:

$A^{m+}_{(12-n-x)/m}B^{n+}X^{2-}_{(6-x)}Y^{-}_{x}$(A: Cu, Ag, Cd, Hg; B: Ga, Si, Ge, Sn, P, As; X = S, Se, Te; Y = CI, Br, I; $0 \leq x \leq 1$). With a disordered A-cation sub-lattice. Transitions into other ordered structures occur at lower temperatures. An anion framework of interpenetrating, centered icosahedra provides ideal and deformed tetrahedral cation sites, which is a characteristic structural property. Some argyrodites work well as ionic conductors, while others work well as non-linear optical materials. Despite the fact that the argyrodites family's structurally similar structures may be observed to arise from a single high-temperature parent phase with (overall) cubic symmetry F43m [14]. Phosphorus-containing argyrodites Me_6PS_5X (Me = Cu+, Ag+, Li+, and X = Cl, Br, I) are now the most investigated compounds Me_6PS_5X and M_6PSe_5X (M=Ag, Cu and X=Halide) belong to a large class of solids collectively referred to as argyrodites. Phosphorus-containing argyrodites Me_6PS_5X (Me = Cu+, Ag+, Li+, and X = Cl, Br, I) are now the most investigated compounds Me_6PS_5X and M_6PSe_5X (M=Ag, Cu and X=Halide) belong to a large class of solids collectively referred to as argyrodites [15]. Thermoelectric materials can convert waste heat to usable electricity. The technology of energy conversions from waste heat into electrical energy is very important for developing alternative energy technologies to reduce our dependence on fossil fuels. The efficiency of a thermoelectric device depends on material properties, which in turn Depend on the thermoelectric figure of merit. Focused on thallium tellurides as advanced thermoelectric materials [16]. Having current scientific interests in the structural family of argyrodites [17, 18]. The compounds Ag_8SiTe_6 and Ag_8GeTe_6 under our consideration form an important group of argyrodites their properties have not been fully investigated experimentally as well as theoretically. It is, therefore, imperative to perform a detailed theoretical investigation of these compounds to understand them and to judge their suitability towards optoelectronics and thermoelectric applications.

2: Computational Details

The structural, electronic, optical and elastics characteristics and properties of the argyrodites A_8BC_6 (A=Ag; B=SI, Ge; C=Te). were investigated by using the method of FP-LAPW [19] with in the DFT framework implemented in the Wien2K code using in material modeling [20] Wu-Cohen-Generalized Gradient Approximation (WC-GGA) [21] the modified Becke-Johnson potential (mBJ) were used to approximate the exchange-correlation potential [22]. To carry out electronic structure the FP-LAPW method is widely used in Wien2K calculation. This method is used to solve the Kohn-Sham's equation for many body systems by this method the unit cell is split into two regions i.e. Moffin Tin region and interstitial region. The potential is considered to be spherically symmetric in Moffin Tin region while in interstitial region considered constant. Plan wave solutions and radial solution of the Schrödinger wave equation are used in the Moffin Tin region and interstitial region respectively inside the sphere. For expansion of wave inside the spheres the maximum value of angular momentum $1_{max} = 10$ is considered. Similarly the plane wave cutoff value $R_{MT}.K_{max}$ =7 is chosen for interstitial region to separate the core and valance states the cutoff energy -6Ry is to be taken to perform Self-Consistent Field (SCF) calculation a k-mesh with 1000 k-points in the first Brillion zone was used.

3. Results and Discussion

3.1. Structural Properties

Compound structural properties are determined by looking at a variety of structural parameters. The structural parameters are the lattice constants a (Å), b (Å), and c (Å), the bulk modulus B (GPa), and the bulk modulus (Bp) pressure derivative. The mention structural characteristics are obtained by maximizing the volume of the unit call of the substance. The total stable state energy was calculated using "Birch Murnaghan's equation of state. The technique of optimization produces the plot between the unit cell volume and the related energy. Ag_8SiTe_6 and Ag_8GeTe_6 are argyrodites with the general formula A_8BC_6 (A=Ag; B=SI, Ge; C=Te). Figure 3.1 shows the crystal structure of Ag_8SiTe_6, which is isostructural with Ag_8GeTe_6. The structure is a cubic crystal with the space group F.43m, and each unit cell contains more than 60 atoms. Ag_8SiTe_6, on the other hand, has the same crystal structure as Ag_8GeTe_6 [16].

3.2. Volume Optimization

The optimizing volume of unit cell and energy is satisfied by Brich Murnaghan relationship.

$$E(V) = E_0 = \frac{9V_0B_0}{16}\{[(\frac{V_0}{V})^{2/3} - 1]^3 - B_0^{/} + [(\frac{V_0}{V})^{2/3} - 1]^2[(6 - 4\frac{V_0}{V})^{2/3}]\}$$

Ground state parameters are represented by Energy (E_0), volume (V_0) and modulus of (B_0) [23].The optimize graph of the two compounds Ag_8SiTe_6 and Ag_8GeTe_6 shown in figure 3.2 (a, b) parabolic curves show the optimize volume of unit cell which similar to ground state density, ground state volume and energy are indicated at the lowest point of parabolic curve the minimum energy state is called the steady state which is the most stable state corresponds to the experimental values. The lattice constant at stable state of both compounds Ag_8SiTe_6 and Ag_8GeT_6 were computed by the optimization of the structure that is 12.130 A^0 and 12.89 A^0 respectively with a very slight variation from experimental ones which is 11.515 A^0 and 11.566 A^0 for Ag_8SiTe_6 and Ag_8GeTe_6[23, 24].

3.3. Electronic Properties

The electronic properties are a set of factors and representations that comprehensively explain the state and behavior of electrons in materials. The electronic properties of Argyrodites A_8BC_6 (A=Ag; B=Si, Ge; C=Te) compounds in cubic phase have been explored using electronic structure of bands and total as well as calculations of partial density of states.

3.4. Energy Band Structure

The energy bands are of two types of a material according to energy band theory the conduction band (CB) and valance band (VB) the area in which electrons are not fit is called prohibited energy band gap which in between the valance and conduction bands. The types of materials also distinguish from band structure whether it is conductors, insulators, or semiconductors. Material having direct band gap used in optical devices. Visible region band gap from $1.3eV$ to $1.8eV$ with a band gaps of $1.4eV$ and $6.0eV$ the material behaves semiconductor and insulator. The overlapping of conduction and valance band at Fermi level show the metal nature of material according to band gap theory. Wu-Cohen, GGA, PBE sol-GGA and modified Becke-Johnson method are used for the study of electronic band structure of argyrodites Ag_8SiTe_6 and Ag_8GeTe_6 in the energy ranges from $-3eV$ to $3eV$ from the band structure of these compounds it is clear that the selected compounds have direct band gap. Ag_8SiTe_6 have semiconductor nature with a band gap of $0.24eV$ while Ag_8GeTe_6 have half metallic nature with a band gap of $0.0068eV$ .The Eigenvalues of VBM, CBM and Fermi energy for Ag_8SiTe_6 are 5.649 eV, 5.890 eV and 5.743 eV.The Eigenvalues of VBM, CBM and Fermi energy for Ag_8GeTe_6 are 5.214 eV, 5.209 eV and 5.209 eV.

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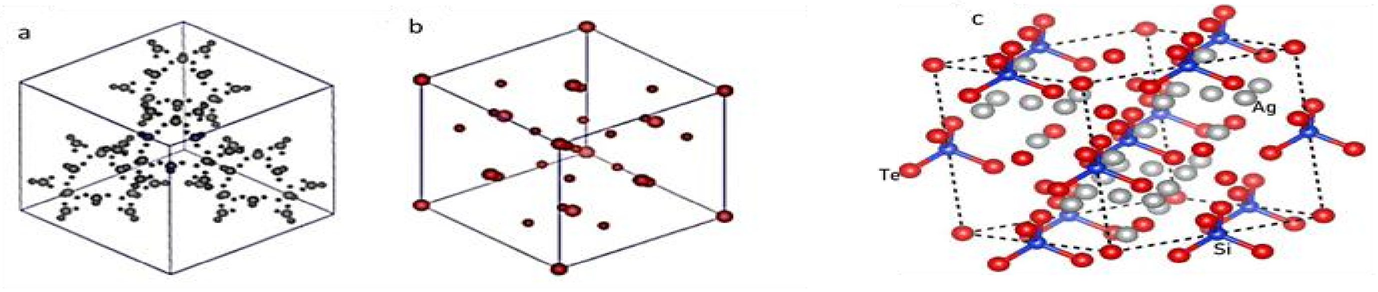

Figure 1: Ag_8SiTe_6 crystal structure. Ag, Si, and Te are represented by grey, blue, and red balls, respectively. Individual places of Ag and Te are indicated by (a) and (b), respectively. (c) Shows the locations of Ag, Si, and Te in the same crystal frame.

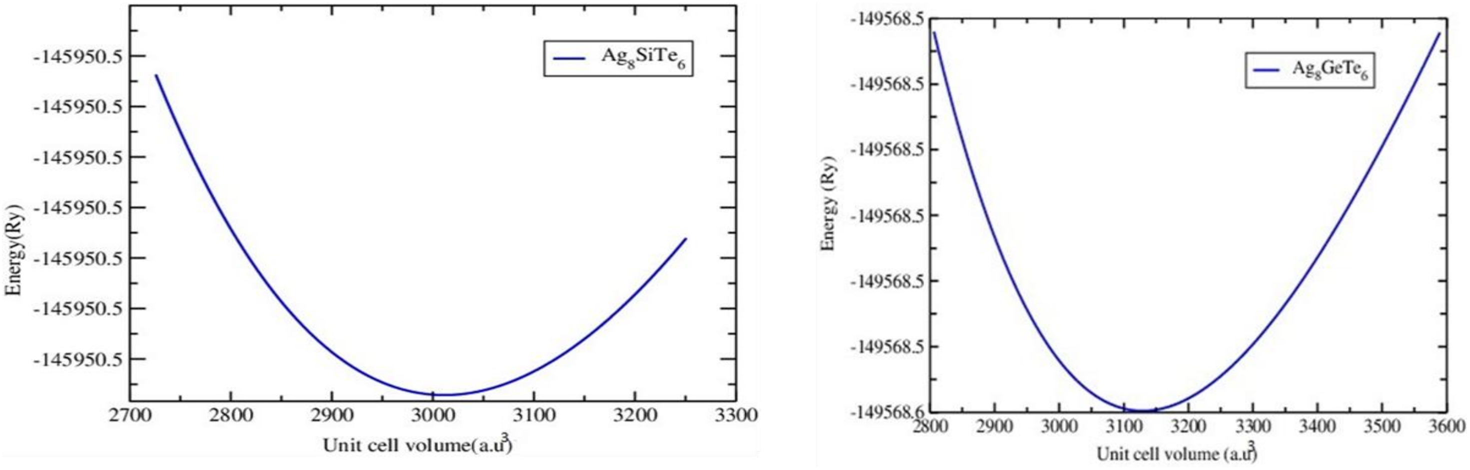

Figure 2: volume optimization of compounds (a) Ag_8SiTe_6 (b) Ag_8GeTe.

Compounds	Lattice constant (A^0)		V_0 (a.u^3)	B(GPA)	Bp	E_0(Ry)
	A^0_{comp}	A^0_{exp}				
Ag_8SiTe_6	12.130	11.515	3011.332	33.697	5.148	– 145950.526
Ag_8GeTe_6	12.289	11.566	3131.189	37.571	7.072	– 149568.559

Table 1: summarizes the lattice constants of stable compounds, as well as their related energies, equilibrium structures, bulk modulus, pressure derivative of bulk modulus, optimized volume, and experimental values.

3.6. Energy Band Structure

The energy bands are of two types of a material according to energy band theory the conduction band (CB) and valance band (VB) the area in which electrons are not fit is called prohibited energy band gap which in between the valance and conduction bands. The types of materials also distinguish from band structure whether it is conductors, insulators, or semiconductors. Material having direct band gap used in optical devices. Visible region band gap from $1.3eV$ to $1.8eV$ with a band gaps of $1.4eV$ and $6.0eV$ the material behaves semiconductor and insulator. The overlapping of conduction and valance band at Fermi level show the metal nature of material according to band gap theory. Wu-Cohen, GGA, PBE sol-GGA and modified Becke-Johnson method are used for the study of electronic band structure of argyrodites Ag_8SiTe_6 and Ag_8GeTe_6 in the energy ranges from $-3eV$ to $3eV$ from the band structure of these compounds it is clear that the selected compounds have direct band gap as shown in figure 3 (a) and 3 (b). Ag_8SiTe_6 have semiconductor nature with a band gap of $0.24eV$ while Ag_8GeTe_6 have half metallic nature with a band gap of $0.0068eV$.The Eigenvalues of VBM, CBM and Fermi energy for Ag_8SiTe_6 are 5.649 eV, 5.890 eV and 5.743 eV.The Eigenvalues of VBM, CBM and Fermi energy for Ag_8GeTe_6 are 5.214 eV, 5.209 eV and 5.209 eV

3.7. Density Of States

In condense matter physics and solid state physics the accessible state per unit energy range occupy by electron is describe through density of state (DOS) different energy levels make the band structure of a substance the band structure consist of valance and conduction band the contribution of different orbitals in the valance and conduction band are explain by DOS plots which is a simple approach to the contribution of orbitals in the band structure for both compounds Ag_8SiTe_6 and Ag_8GeTe_6 the energies are distributed between $-6eV$ and $6eV$ as illustrated below. For Ag_8SiTe_6 the total density of state (TDOS) is show in the figure 4 (a) the contribution of Ag atom maximum to the TDOS in the conduction band as well in valance band and Te atom also have maximum contribution and Si atom have least contribution .TDOS of the compound Ag_8GeTe_6 as show in the figure 4 (b) in which the maximum contribution came from the Ag atom to the total density of state (TDOS) while the other atoms have minimum contribution to the TDOS of the compound Ag_8GeTe_6

3.8. Partial Desity Of States

The partial density of state (PDOS) of the compound Ag_8SiTe_6 is shown in figure 5.1 (a, b, c). In the case of the Ag atom, the partial density of state shown in figure 5.1 (a), the d_{xy} orbital has the maximum contribution to the total DOS of Ag atom in the valance band (V.B), while the s orbital has the maximum contribution in the conduction band (C.B), and the other orbitals have a small contribution to the total DOS of Ag atom. In case of Si atom the partial density of state shown in the figure 5.1 (b) in which p_y orbital have maximum contribution to the total density of states of Si atom in valance band (V.B) while in conduction band (C.B) the maximum contribution came from s and p_x orbital while the other have small contribution to total density of state of Si atom in conduction band.in case of Te atom the partial density of state shown in the figure 5.1 (c) in which p_y orbital have maximum contribution to the total density of states of Si atom in valance band (V.B) while in conduction band (C.B) the maximum contribution also came p_x orbital while the other have small contribution to total density of state of Te atom in conduction band. figure 5.2 (d, e, f) show partial density of state (PDOS) of compound Ag_8GeTe_6.in case of Ag atom the partial density of state shown in the figure 5.2 (d) in which $d_z{}^2$ orbital have maximum contribution to the total density of states of Ag atom in valance band (V.B) the contribution of d_{xz} orbital also came maximum in valance band while in conduction band (C.B) the maximum contribution came from s orbital and the other have small contribution to total density of state of Ag atom.in case of Ge atom the partial density of state shown in the figure 5.2 (e) in which p_z and p_x orbital have maximum contribution to the total density of states of Ge atom in valance band while in conduction band from 0 to nearly 1.9eV the maximum contribution came from s orbital and from 2eV to 5eV the maximum contribution came from p_z orbital while the other have small contribution to total density of state of Ge atom in conduction band.in case of Te atom the partial density of state shown in the figure 5.2 (f) in which p_z and p_x orbitals have maximum contribution to the total density of states of Ge atom in valance band (V.B) also in conduction band (C.B) the maximum contribution came from p_x and p_z orbitals while the other have small contribution to total density of state of Te atom in conduction band.

4. Optical Properties

The response of materials to the electromagnetic radiation shows the optical properties of materials. Argyrodites Ag_8SiTe_6 is semiconductor and Ag_8GeTe_6 is half metallic so the optical parameters such that complex dielectric constant, refractive index, reflectivity, optical conductivity, absorption and extinction coefficient energy/frequency dependent optical properties determined with detail explanation when the material expose to electromagnetic radiation. For the study of optoelectronic applications, we need a detail information about material response to visible, infrared and ultra violet radiations.

4.1. Real And Imaginary Dielectric Functions

The dielectric function descried the response of materials when expose to electromagnetic radiation Dielectric function have two parts real and imaginary complex dielectric function can be written as $:\mathcal{E}(\omega) = \mathcal{E}1(\omega) + i\mathcal{E}2(\omega)$ real part $\mathcal{E}1(\omega)$ is responsible for the material how much material disperse light or how much the material polarizibility while the imaginary part $\mathcal{E}2(\omega)$ show the material absorption properties. In the band structure different transitions of orbitals the argyrodites compounds Ag_8SiTe_6 and Ag_8GeTe_6 shows different optical spectra's Ag_8SiTe_6 semiconductor in nature so the optical properties will different as compare Ag_8GeTe_6 to have half metallic nature illustrated in figure 6 (a) Static dielectric constant $\mathcal{E}1(0)$ is called zero frequency limit. Ag_8SiTe_6 has a static dielectric 13.0 in the energy ranges from 0 to $0.5eV$ the polarizibility increasing when the photons energy increases the maximum spectra for Ag_8SiTe_6 compound will be occur at energy $1.81eV$ is 16.7 after reached to this maximum peak the disperse light now decreasing and reached to its minimum point below zero point in the negative region the metallic nature of material indicated. Compound Ag_8GeTe_6 shows half metallic nature in band structure so spectral lines varies with the photon energies illustrated in the figure 6 (a) static dielectric function is in the energy ranges from 0 almost to $0.9eV$ the critical point is at 14.70 at energy $0.04eV$ the maximum dispersion of the Ag_8GeTe_6 at energy 1.44 eV is 16.80 after the maximum peak dispersion decrease with the increasing in energy and become negative at a specific energy.

Imaginary part $\mathcal{E}2(\omega)$ of the dielectric function for compounds Ag_8SiTe_6 and Ag_8GeTe_6 the figure illustrated in 6 (b) shows the absorption properties of silver based argyrodites materials the spectra threshold points of the materials related with the band gap energy beyond the threshold point different curves causes by inter band transitions critical point for Ag_8SiTe_6 occur at energy 0.0605 eV while maximum is at 2.82 eV is 15.7 for Ag_8GeTe_6 and for critical point is at $0.0355eV$ and that of maximum is at $2.59eV$ is 14.9

4.2. Absorption Coefficient $\alpha(\omega)$

The interaction between the incident photon on material surface and the absorption of photon in the material surface illustrated in figure 7 (a, b) of the absorption $\alpha(\omega)$ the critical points are at energies 0.280 eV and 0.157 eV for both compounds Ag_8SiTe_6 and Ag_8GeTe_6 the absorption coefficient increasing as the photon energy increasing the peak values of absorption coefficient $\alpha(\omega)$ for Ag_8SiTe_6 is 1.3×10^6 cm^1, at energy 7.84 eV and for Ag_8GeTe_6 is $1.3\times 10^6 \text{cm}^{-1}$ at energy 7.3.

4.3. Extinction Coefficient $K(\omega)$.

Extinction coefficient indicate the absorption of photons by material. The extinction coefficient is a measure of the attenuation of an electromagnetic wave as it passes through a material. It is a measure of the rate of decrease in transmitted photons due to scattering and absorption for a medium.

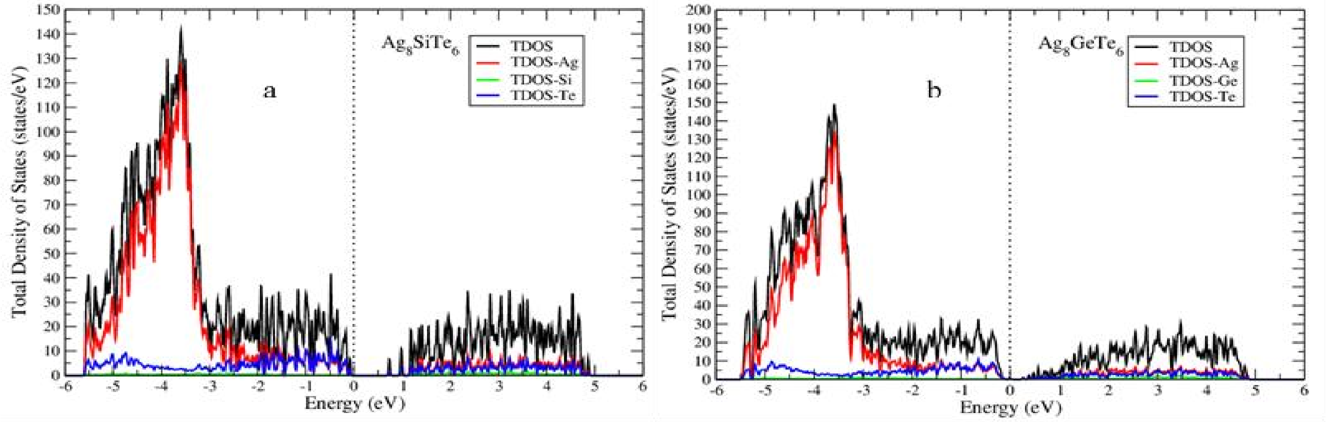

Figure 3: Energy band structures (a) Ag_8SiTe_6 (b) Ag_8GeTe_6

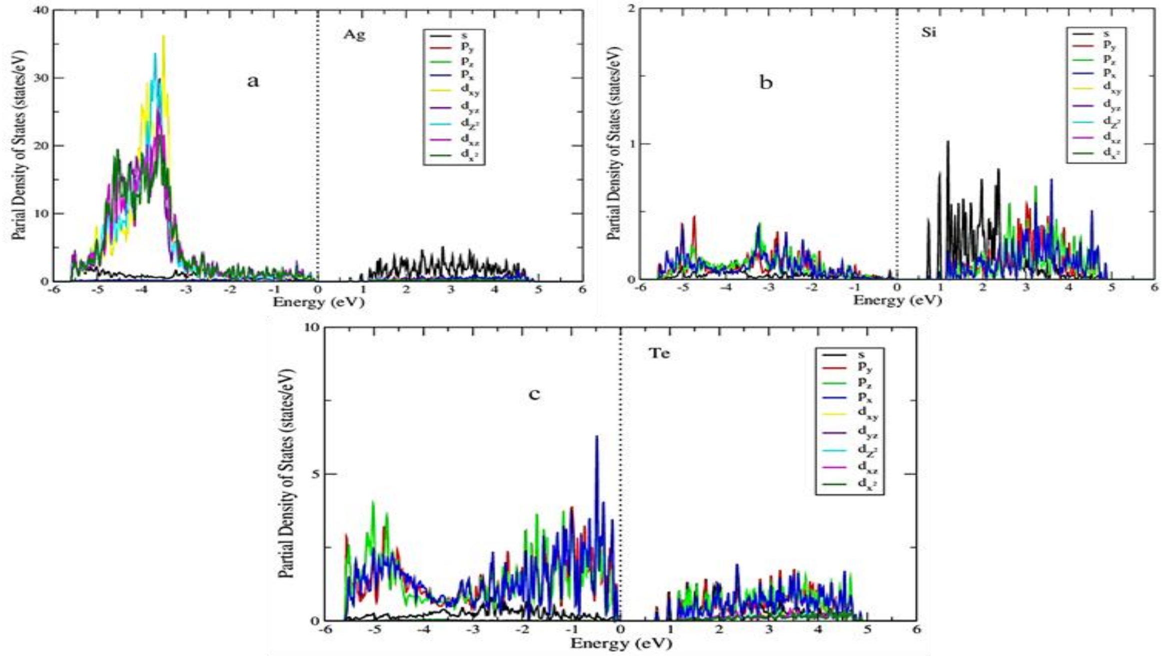

Figure 4: (a) and (b) shows the Total density of state (TDOS) of compound Ag_8SiTe_6 andAg_8GeTe_6

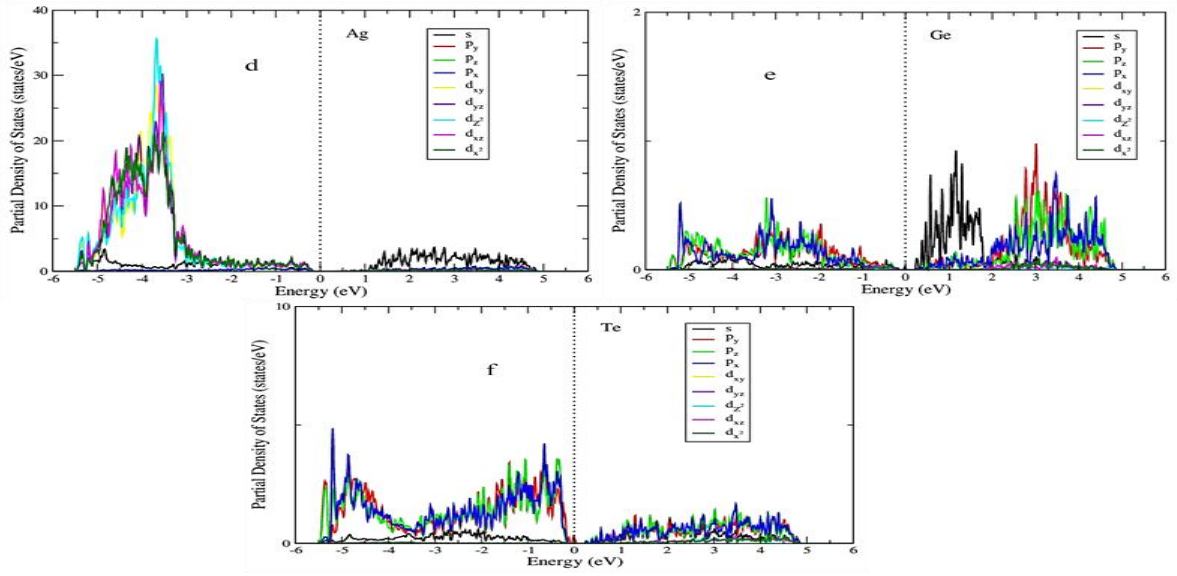

Figure.5.1: Partial density of state (PDOS) of compounds Ag_8SiTe_6

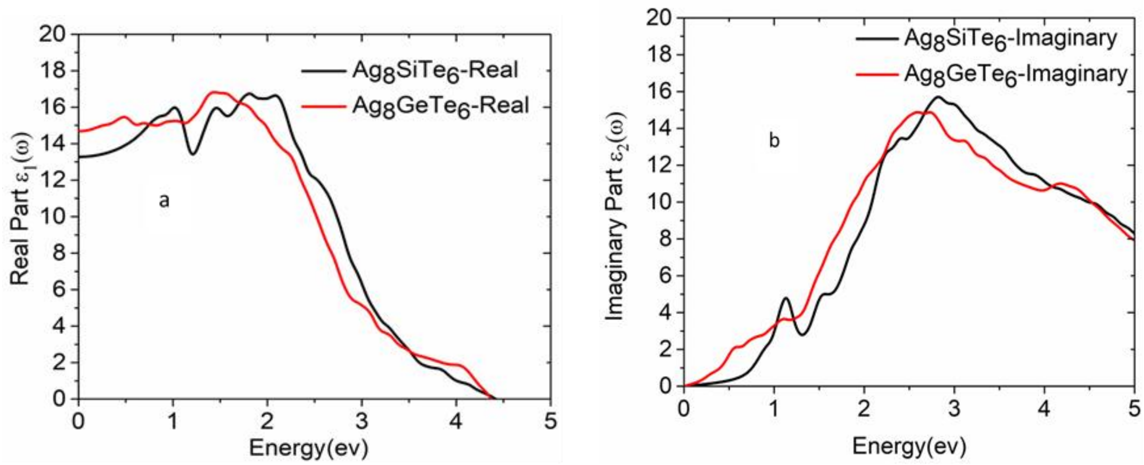

Figure 6: (a) real part $\mathcal{E}1(\omega)$ and (b) imaginary part $\mathcal{E}2(\omega)$ of dielectric function for compounds Ag_8SiTe_6 and Ag_8GeTe_6

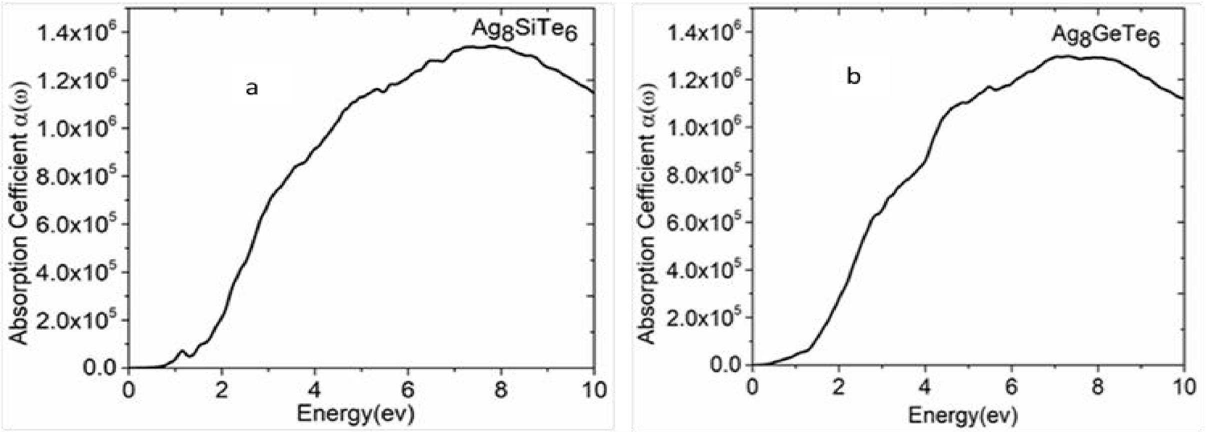

Figure 7: The absorption coefficient $\alpha(\omega)$ of compounds (a) Ag_8SiTe6 (b) Ag_8GeTe_6

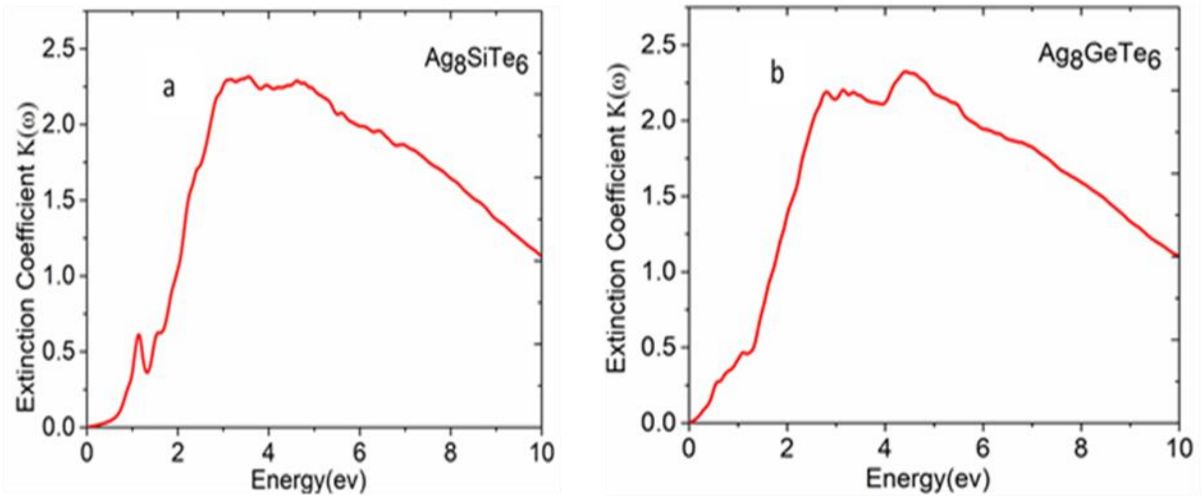

Figure 8: shows the extinction coefficient $K(\omega)$ of compounds (a) Ag_8SiTe_6 (b) Ag_8GeTe_6

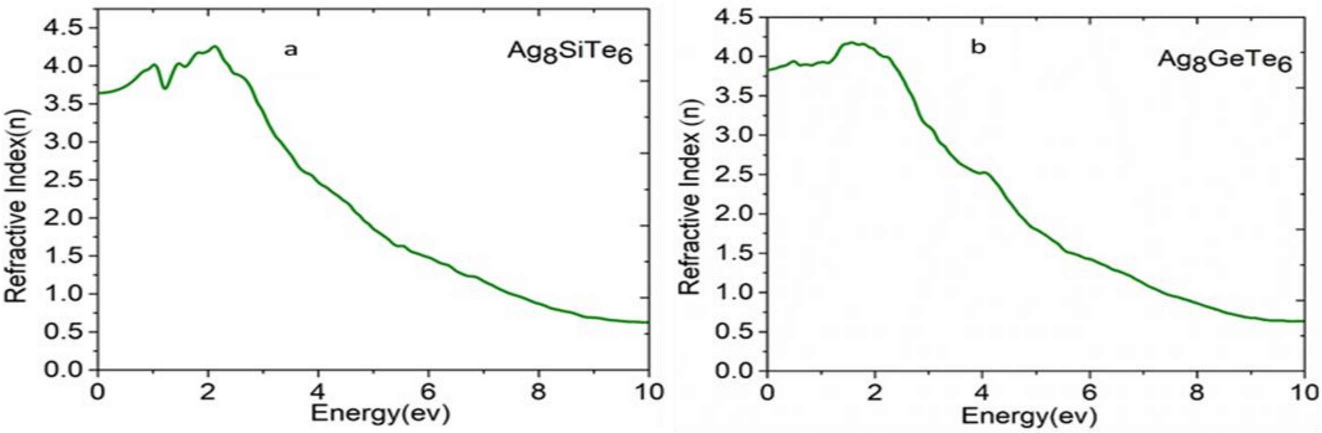

Figure 9: The refractive Index (n) of compounds (a) Ag_8SiTe_6 (b) Ag_8GeTe_6

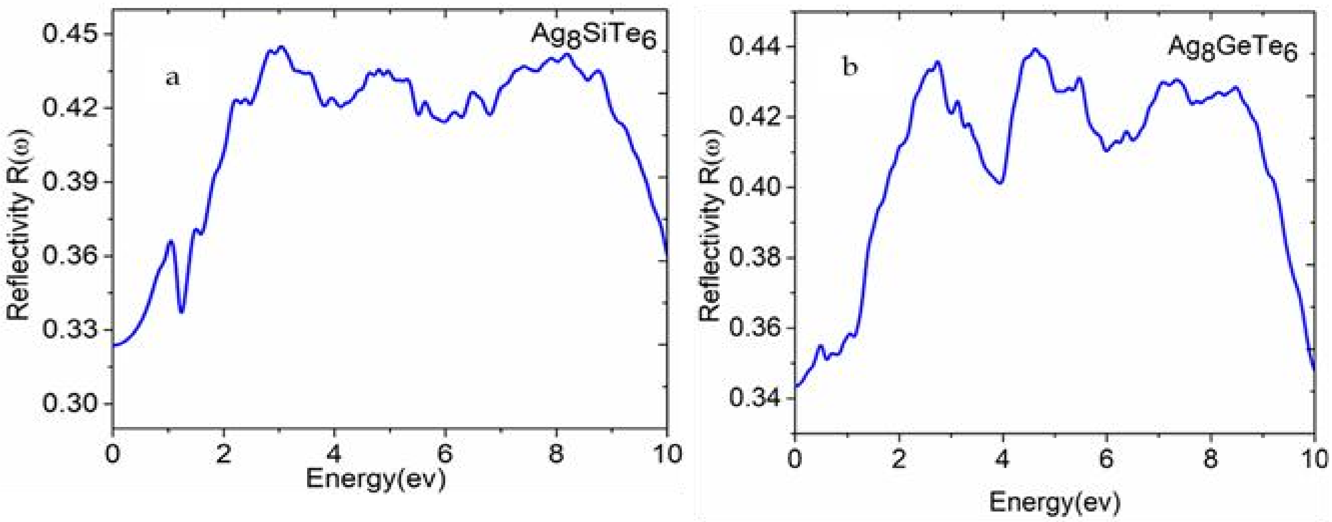

Figure 10: The Reflectivity $R(\omega)$ of compounds (a) Ag_8SiTe_6 (b) Ag_8GeTe_6

Table 2: Electron and hole effective mass of compounds Ag_8SiTe_6 and Ag_8GeTe_6

Compounds	Effective mass(me*) of electron Kg	Effective mass(mh*) of hole Kg
Ag_8SiTe_6	$0.65x10^{-32}$	$-3.78x10^{-32}$
Ag_8GeTe_6	$1.39x10^{-32}$	$-2.15x10^{-32}$

This is because the refractive index is complex and can be express as n-iK. Where n is the real part of the refractive index (which tells the velocity in the medium) and K is the extinction coefficient. The extinction coefficients of the Ag_8SiTe_6 and Ag_8GeTe_6 compounds are illustrated in figure 8(a, b). The maximum value of $K(\omega)$ for the Ag_8SiTe_6 compound is 2.32 at energy of 3.56 eV, and for the Ag_8GeTe_6 compound an extinction coefficient of 2.32 at an energy of 4.41 eV, respectively, is observed. The extinction coefficient $K(\omega)$ is a measure of light loss due to scattering and absorption per unit volume, so the value of $K(\omega)$ is high

4.5. Refractive Index (n)

The propagation of light through material medium is explain by refractive index .Speed of light is represented by c and refractive index is by n The optical transparency of any material can be investigated through refractive index, extinction and absorption coefficient of electromagnetic radiation refractive index as show in the figure 9 (a, b) is 3.64 at zero frequency and at energy 0.026 eV for compound Ag_8SiTe_6 while maximum peak will be 4.26 at 2.12 eV due to energy increasing the refractive index fluctuation between 3.64 and 4.26 in the energy ranges from 0.026 eV to 2.12 eV. For compound Ag_8GeTe_6 in the energy range from 0.016 eV to 1.571 eV, the refractive index n fluctuates between 3.83 and 4.181 due to the various rates of the inner-band transitions the lower refractive index indicates less polarization in the higher energy range for both compounds the fall of refractive index (n) suggested the reduction of magnetization with increase in energy

4.6. Reflectivity $R(\omega)$

Ratio between incidents, reflected light called coefficient of reflectance or reflectivity behavior of electromagnetic radiation on the surface of material is described by the interaction of EM radiation to the material surface. Material surface properties and material surface information is described by this important property energy ranges is in between 0 to 10 eV for both compounds Ag_8SiTe_6 and Ag_8GeTe_6 show in the figure 10 (a, b) in figure (a) the lowest value at which just both compound Ag_8SiTe_6 start is called zero photon energy or critical point that is 0.342 at energy 0.0206 eV between the energy ranges reflectivity $R(\omega)$ increases at energy $1.04\,eV$ is 0.336 and then decreases to 0.337 at $1.23\,eV$ and then gain a spectacular peak of 0.445 at energy $3.03\,eV$ can be detected and then reflectivity start decreasing with the increasing of energy in figure (b) for compound Ag_8GeTe_6 zero photon energy or critical point start from 0.0057 at energy 0.034 eV and continue to increase up to 0.355 at energy 0.496 eV then decreases at energy 0.641 eV to 0.351 at energy 4.42 eV a remarkable peak of 0.493 seen in the reflectivity after thisstart decreasing to its minimum values a significant lower values is observe between 0.496 eV to 0.641 eV.

5. Effective Mass

To comprehend the concept of effective mass, we must first comprehend the band structure in solids, where energies are dispersed in two types of energy bands: valence band and conduction band. The curvature of E-K relationships determines the effective mass (m*) of curvature in a semiconductor. Energy (E) and wave vector K have a parabolic relationship. By comparing each electron's behavior to that of a free particle of the same mass, the effective mass (m*), energy (E), and wave vector (K) are computed. Effective mass is represented as by making an analogy with the behavior of a free particle of that mass. $m_e^* = \hbar^2[\frac{d^2E}{dk^2}]^{-1}$. By using the band structure of silver argyrodites compounds A_8BC_6 (A=Ag; B=Si, Ge; C=Te), the effective mass is determined by measuring the curvature of conduction band minima. The estimated hole impact mass mh* is negative due to valence band minima. The negative number indicates that if a force is applied in the -X direction, the electron will move in the +X direction like electrons in lattice as a result holes move in a semiconductor with an effective mass that is generally negative near the band's top, according to band-structure calculations. The hole effective mass is smaller than electron effective mass

6. Conclusions

Through the study of computational analysis, the structural, electronic and optical properties of A_8BC_6 (A=Ag, B=Si, Ge, C=Te) argyrodites compounds were generated using the FPLAPW method using the mBJ approximation implemented in the wien2k code. Structural optimization of A_8BC_6 argyrodites (A=Ag; B=Si, Ge; C=Te) shows that the lattice parameters and bulk modulus of the A_8BC_6 compound are substantially close to the available experimental data. The electrical properties of the A_8BC_6 argyrodites compounds show a straight band gap behavior. Ag contributes the greatest to the overall density of states in the valence band in these compounds. The optical properties of the A_8BC_6 (A = Ag; B = Si, Ge; C = Te) argyrodites compound are determined from the results of the complex dielectric function, refractive index, extinction coefficient, photoconductivity, absorption coefficient, and reflectance. All peaks (maximum values) in the absorption spectrum of the A_8BC_6 compound are due to inter band transitions of electrons. The optical properties of these materials were calculated in the energy range from 0 to 10 eV. The absorption coefficient increases as the energy of the incident light (photons) increases. The coefficient of absorption increases as the energy of the incident light (photon) increases. The maximum value in the real and imaginary part of the complex dielectric function are found at energies of 1.81 eV for Ag_8SiTe_6 and 1.44 eV for Ag_8GeTe_6. The critical points of these substances are found in the visible spectrum on an absorption coefficient. For compound Ag_8SiTe_6 absorption start from 0.28 eV up to maximum point of 7.84 eV and for Ag_8GeTe_6 absorption start from 0.157 eV up to maximum point of 7.31 eV which shows the absorption of ultra violet spectrum which is from 3.1 eV to 30 eV

Authors Contribution

Muhammad Munsif, Matiullah Shah and G.Murtaza have the main idea of the manuscript and wrote the manuscript. Suliman Khan ,Asim Sajjad, Zakir Ullah, Hamid Ullah and Abdur Rashid revised the manuscript and provide suggestions.

Conflicts of Interest

The authors reported no potential conflict of interest.

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Data Availability statement

The data presented in this study are available on request from the corresponding author.

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