Accepted manuscript (author version)

**To appear in: International Journal of Nano Dimension (Int. J. Nano Dimens.)**
Online ISSN: 2228-5059 Print ISSN: 2008-8868

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Received: 24 June 2024 Revised: 29 Aug. 2024

Accepted: 10 Sept. 2024

**DOI: 10.57647/ijnd-2024-sf9q**

**Original Article**

# First-principles calculations to investigate electronic, optical and thermoelectrical performances of Pb/Te-based nanolayer and bulk chalcogenides

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## Abstract

The electronic,thermoelectricand optical properties of bulk and nanolayers chalcogenides, specifically XTe (X = Si, Ge, Sn, and Pb) and PbY (Y = O, S, Se, and Te), have been investigated using density functional theory (DFT) with the GGA-PBE functional and semiclassical Boltzmann theory via Quantum ESPRESSO and BoltzTraP codes. The results of the electronic band structure analysis indicate that compounds such as PbO, PbS, PbSe, PbTe and GeTe exhibit direct band gaps, making them suitable for semiconductor applications. On the other hand, SiTe and SnTe



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compounds exhibit metallic behavior. Also, the GeTe bulk was converted from semiconducting to conducting in the nanolayer structure. The thermoelectric properties of these bulk and nanolayerschalcogenides, including electrical conductivity, electronic thermal conductivity, and Seebeck coefficient, have been calculated. It was observed that the Seebeck coefficient decreases with increasing temperature in all semiconductor samples. Moreover, the thermal and electrical conductivity coefficients increase with the increase in chemical potential, transferring it to the electrons in the conduction layer. Based on the findings, it can be concluded that PbTe shows promising potential as a candidate material for thermoelectric devices. Seebeck coefficient in PbO, PbS, and PbSe nanolayers increased compared to the bulk structure. The optical properties, including the real and imaginary parts of the dielectric function, absorption, and reflectivity as a function of energy, have also been calculated. The absorption edges of the bulk chalcogenides extend into the visible spectrum due to their suitable bandgap values. Additionally, these materials exhibit non-transparency in certain regions of the electromagnetic spectrum, making them suitable for use as absorbent materials. Among the chalcogenides studied, PbS shows promising potential for optoelectric industries due to its low refractive index and high optical gap. Also, the decrease in the refractive index of the nanolayers compared to the bulk shows more optical absorption in them. Additionally, among bulks compounds, PbTe shows promising potential for thermoelectric applications, while among nanolayers, PbO is the most suitable material.

**Keywords:** *DFT*; *Nanolayers; Optical properties; Pb-based chalcogenides; Te-based chalcogenides; Thermoelectric properties.*

## 1. Introduction

Today with the progress in nanotechnology, in the context of increasing energy demand, exhaustion of fossil fuels, and global warming, renewable energy sources are becoming increasingly important; these energy sources are clean, sustainable, and can be exploited for thousands of years [1-4]. Among the various types of renewable energy options, such as wind, solar, hydro, and geothermal energy, thermoelectricity is the most environmentally friendly [5]. Thermoelectricity is the field of science that encompasses energy conversion; it converts heat into electrical energy (Seebeck effect) or vice versa, electrical energy into heating or cooling (Peltier effect) [6-8]. Among these two effects, the conversion of heat into electrical energy offers a way to store wasted thermal energy, which has the advantage of being stored in a smaller space for longer periods of time. Given these benefits, researchers are working to develop materials and nanomaterials that exploit the Seebeck and Peltier effects to extract free, wasted, and renewable energy. This article discusses the extraction of electrical power from waste heat using thermoelectric materials. The fundamentals of the Seebeck effect are also described, along with recent



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developments in thermoelectric energy conversion with an emphasis on the Peltier effect [6-8]. Additionally, recent research on new materials with various structures (bulk, nanolayer, nanoparticle, nanotube and thin film) for thermoelectric (TE) energy conversion is discussed. The need for high TE efficiency with low engineering costs poses the major challenge in this area. Until now, TE energy extraction was hampered by several factors such as toxicity, low efficiency, and limited availability of certain chemical elements. TE materials should be able to generate the appropriate voltage with arbitrary temperature differences in order to convert heat into electricity. For this purpose, the electrical conductivity ($\sigma$) and Seebeck coefficient (S) should be high so that the thermal noise is extremely low. Moreover, the electronic ($\kappa_e$) and lattice thermal conductivity ($\kappa_l$) should be kept as low as possible to ensure minimal loss of thermal energy. In this article, these properties are examined with the help of the figure of merit, ZT [9-11].

$$ZT = \frac{\sigma S^2 T}{\kappa_e + \kappa_l} \quad (1)$$

At present, almost all of the TE materials have a low ZT value, which is less than 1. This has led to the development of new semiconductors with higher ZT values as the main direction of TE materials research [12-20].

This is because TE materials with a ZT value greater than 1 open up new development directions for the application of TE materials in various industries. The most promising thermoelectric materials are mainly two types: semiconductor alloys and chalcogenides. These materials can be selected according to the temperature range required for applications at any temperature, and finally, a comprehensive decision is made base on the performance [21-25]. For applications at ambient temperatures above 150 °C, a variety of TE devices based on bismuth telluride (BiTe) materials have been produced [21-25]. For applications in the medium temperature range of 150-500 °C, a variety of TE devices based on lead telluride (PbTe) materials were produced [26-30]. For medium temperatures above 500 °C, a variety of TE devices based



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on silicon germanium (SiGe) materials were produced [30-34]. In recent years, a large number of minerals, organic and phase hybrid TE materials have been reported in the literature to prepare TE devices [35-43]. Among inorganic TE materials, minerals such as $Bi_2Te_3$, SiGe, PbTe and their alloys exhibit the highest ZT coefficient [44]. For example, the resulting compound Bi2Te3 has a ZT value of 0.8 to 1.0 and room temperature (T=300 K) [45]. Early on, research was conducted on how to improve the Seebeck coefficient (S) and electrical conductivity (σ) of tellurium-based chalcogenide TE materials in order to achieve the target ZT [46]. For example, researchers found that PbTe achieves ZT values of 1.4, 1.5 and 1.8 at temperatures of 750, 773 and 850 °K, respectively [47-49].

Mishra *et al.* [50] consider the electronic and TE properties of boron chalcogenide materials BX (X = S, Se, Te) and found that these materials have a good value of ZT close to unity for the temperature range of 200-450 K. The highest value of ZT is about 1.022 in the case of BSe. Also, Gupta *et al.* [51] investigate the TE properties of the chalcogenide material SnSeS and its defect using the first principle approach in medium temperature range (300-800 K). In this range, they found that $SnSe_{0.7}S_{0.3}$ has the highest ZT [51]. Chalcogenide semiconductors have a significant optical response and are also quite useful for solar cell and infrared detector applications. However, the optical behavior of the solids is related to all the electrons in the materials and not only the free electrons. The dielectric function is an experimental function that is very sensitive to the crystal band structure and hence can be utilized to find out the overall crystal band structure. Several studies are available in the literature, and in the last few years, many articles have been reported on the optical behavior of chalcogenide compounds in different structures [52]. These studies contribute a lot in understanding the optical behavior, future and potential applications for these applications. Azam *et al.* [53] calculated the optical properties of ternary chalcogenides $AlX_2Te_4$ (X = Zn, In) using Density Functional Theory (DFT) in the energy range of 0 to 14 eV. Their results indicated that these materials could be a suitable choice for optoelectronic devices. Mathew *et al.* [54] investigated the optical properties of $BaTiX_3$ (X = S, Se) using DFT+U. Their findings revealed that both materials exhibit significant optical anisotropy for various values of U. Goumri-Said *et al.* [55] studied



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the optical properties of ternary selenide chalcogenide $Tl_3AsSe_3$ using the Modified Becke Johnson (mBJ) approximation. The results of their research demonstrated that this material maintains a positive refractive index, indicating a non-negative refractive index value. Challenging semiconductors have attracted the attention of researchers mainly because of their unique thermoelectric and optical properties. Pb/Te-based chalcogenides have long been known as diverse functional materials and are of interest in nano chemistry today. New and innovative synthesis methods of these compounds in the form of nanowires, nanolayers and nanocrystal networks turn them into materials with interesting and unpredictable properties [56-63].

In this paper, the authors conducted a comprehensive study on the structural, electrical, thermoelectric and optical properties of three-dimensional (bulk) and nanolayers chalcogenides XTe (X=Si, Ge, Sn and Pb) and PbY (Y=O, S, Se, and Te) materials. The nanolayers studied in this article are all monolayers. The investigation was carried out using DFT with the GGA-PBE functional, as well as semiclassical Boltzmann theory through the utilization of Quantum ESPRESSO and BoltzTraP codes. This study represents the first exploration of these properties for the mentioned materials. These nanolayers have many applications in infrared sensors, military industries, optical filters and ultraviolet absorbers.

**2. Computational details**

In this article, the properties of XTe and PbY materials were calculated using the DFT method and the Quantum Espresso (QE) simulation code [64]. The self-consistent calculations (SCF) were performed using the pw.x code from the QE code packages. The parameters used for the SCF calculations included a K-point grid of 12×12×12, an energy convergence limit of $10^{-8}$ Ry, and a convergence threshold on forces of $10^{-5}$ Ry/$a_0$. The kinetic energy cutoff for wave functions and charge density was set to approximately 30 and 300 Ry, respectively. The projected augmented-wave (PAW) pseudopotentials were utilized for the exchange-correlation term in the PBE method [65]. Ultrasoft (USPP) pseudopotentials were employed in all calculations. For the calculations of the electronic band structure, density of states (DOS) and projected density of states (PDOS), the band.x, dos.x and projwfc.x codes were used, respectively.



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Optical calculations were performed using a larger mesh of 20×20×20 k-points and the epsilon.x code. The thermoelectric properties of the compounds were obtained using the BoltzTrap computational code, which utilizes the semi-classical Boltzmann method. For this purpose, a bulk network with a specified number of wave vector points (20 × 20 × 20) was employed.

## 3. Results and discussion

### 3.1. Structural and stability properties

The bulk chalcogenides, XTe (X = Si, Ge, Sn, and Pb) and PbY (Y = O, S, Se, and Te), have a cubic (FCC) structure with a primitive unit cell. For all the bulk chalcogenides, the primitive cell contains one Pb/Te atom and one other (X/Y) atom, see Figure 1 for the optimized structures of the bulk chalcogenide materials in both the primitive (a) and the conventional (b) unit cells. To determine the equilibrium lattice constant and the coherence energy, the structures were optimized; see Table 1. In the cubic structure, the Pb and Te atoms are positioned at the center of the cube, while one of the X/Y atoms is placed on each face of the cube. The bond length and the atom angles for the materials in both the primitive and the conventional unit cells are given in Table 2. The formation energy of materials indicates their stability. The higher it is, the higher the stability of the materials. The amount of this energy for SiTe, GeTe, SnTe, PbTe, PbSe, PbS, and PbO in nanolayer mode is 14.6426, 14.4522, 14.1343, 14.1974, 7.2355, 7.7503 and 9.7485 eV respectively. The formation energy of SiTe, GeTe, SnTe, PbTe, PbSe, PbS, and PbO in bulk mode is 13.43, 13.75, 12.95, 13.06, 5.61, 6.65, and 8.47 eV, respectively.

### 3.2. Electronic properties

The band structure was calculated along the symmetric (Γ-W-L-Γ-X-W-K) path of the first Brillouin zone of the primitive cubic (FCC) structures to examine the electronic properties of bulk Pb/Te-based chalcogenides. The calculated band structures are shown in Figures 2(a-d) and 3(a-d). Fig. 2 shows



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Electronic band structure of a)PbO, b)PbS, c)PbSe, and d) PbTe bulk chalcogenides. In the case of the PbO material (Figure 2(a)), the top of the valence band is around the L point, and the bottom of the conduction band is around the L point, implying that the PbO compound is a direct semiconductor with an energy band gap of 0.17 eV. Similarly, it is found that PbS, PbSe, and PbTe chalcogenides are direct band gap materials when we calculated the band structure along the symmetric L-L path. The obtained energy band gaps for PbS, PbSe, and PbTe compounds are 0.75, 0.57 and 0.85 eV, respectively. Fig. 3 shows Electronic band structure of a) SiTe, b) GeTe, c) PbTe, and d) SnTe bulk chalcogenides. The valence band intersects the Fermi energy in the case of SiTe and SnTe materials (Fig. 3a and 3d), showing its metallic character. Among this group, GeTe chalcogenide has the value of 0.5 eV energy gap. There are only slight differences in these energy gap values when compared with the earlier studies given in the references [66-69]. The density of electronic states (DOS) for XTe (X = Si, Ge, Sn and Pb) and PbY (Y = O, S, Se and Te) bulk chalcogenides are presented in Figures 4(a-d) and 5(a-d). Fig. 4 shows Density of electronic states of a) PbO, b) PbS, c) PbSe, and d) PbTe bulk chalcogenides. Fig. 5 shows Density of electronic states of a) SiTe, b) GeTe, c) PbTe, and d) SnTe bulk chalcogenides. It is seen from these figures that the number of electron states around the Fermi level is completely in accordance with the energy levels of the band structure of these materials from Figures 2 and 3. From Fig. 5(a-d), it is also seen that the density of states around the Fermi band is crossing and it supports the metallic feature of SiTe chalcogenide. Also, PbO, PbS, PbSe, and PbTe nanolayers have energy gaps of 1.367, 0.706, 0.509 and 0.257 eV, respectively [70]. SiTe, GeTe, and SnTe nanolayers are characterized by the absence of energy gaps, rendering them as metallic materials [70]. Wherever there is a gap between the electronic bands, this gap is also observed in the density of states. Therefore, the results of DOS confirm the results of band structure.

### 3.3. Thermoelectric properties



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In the analysis of Thermoelectric (TE) properties, key parameters include electrical conductivity (σ), thermal conductivity (κ) and Seebeck coefficient (S). To determine these coefficients, we utilized the Boltztrap computational code and semi-classical Boltzmann theory [71]. The TE parameters were calculated in the energy range of -2 to 2 eV and at temperatures of 300, 600, and 800 K. Figures 6(a-d) and 7(a-d) depict the Seebeck coefficient (S) of bulk chalcogenides, XTe (X = Si, Ge, Sn and Pb) and PbY (Y = O, S, Se and Te), as a function of the chemical potential. Fig. 6 shows Seebeck coefficient of a) PbO, b) PbS, c) PbSe, and d) PbTe bulk chalcogenides. Fig. 7 shows Seebeck coefficient of a) SiTe, b) GeTe, c) PbTe and d) SnTe bulk chalcogenides. The most significant range of calculated S values is observed in the energy range of -0.5 to 0.5 eV, which is in close proximity to the Fermi level. As the energy moves away from the Fermi level, the S coefficient decreases and approaches zero. Furthermore, the figures demonstrate that the S coefficient decreases with increasing temperature. These findings indicate that these semiconductor compounds exhibit good thermal efficiency. The value of the Seebeck coefficient is positive over the measured temperature range, which shows p-type behavior, and it decreased with the increase of temperature. This value is negative in n-type behavior and decreased with increased of temperature. This opposite behavior is due to Seebeck effect, that temperature and S coefficient have opposite relation ($S=\Delta V/\Delta T$).

The chemical potential (μ) values provide information about the type of charge carriers present. When the chemical potential is positive, it indicates the presence of electron (n) carriers. Conversely, when the chemical potential is negative, it suggests the presence of hole (p) carriers. In all samples, there is a symmetrical behavior observed between holes and electrons for the Seebeck coefficient (S) around the Fermi surface. In the case of SiTe and SnTe chalcogenides, the increase in the density of electronic states around the Fermi level leads to the interference of conduction layer electrons with the Fermi surfaces. This interference results in a decrease in the S coefficient. Negative values of S correspond to n-type (electron) carriers, while positive values correspond to p-type (hole) carriers.



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The highest value of the Seebeck coefficient among lead-based chalcogenides is observed in the PbTe compound. This can be attributed to its larger energy gap compared to other compounds. On the other hand, SiTe and SnTe compounds exhibit the lowest S coefficient values, likely due to their metallic behavior. Table 3 provides a comparison between the current study and previous research on S coefficient and energy gap values for Pb/Te-based chalcogenide nanolayers. The variation in the energy gap significantly affects the thermoelectric properties. The results of this comparison show that PbO, PbS and PbSe nanolayers have a higher S coefficient than their bulk state. This shows that by decrease and changing the dimensions of the material from bulk to nanolayer, due to surface effects, the thermoelectric properties are improved.

In Figures 8(a-d), and 9(a-d), the electrical conductivity (σ) of lead-based and tellurium-based chalcogenides is shown as a function of the chemical potential, respectively. Fig. 8 shows Electrical conductivity of a)PbO, b)PbS, c)PbSe, and d)PbTe bulk chalcogenides. Fig. 9 shows Electrical conductivity of a)SiTe, b)GeTe, c)PbTe, and d)SnTe bulk chalcogenides. Unlike the S diagrams, the electrical conductivity exhibits similar behavior at all temperatures. From these figures, it can be concluded that the values of σ increase with an increase in the chemical potential (μ) in both the negative and positive regions. As μ increases, the density of charge carriers also increases, resulting in an increase in the conductivity of the material.

Figures 10(a-d), and 11(a-d) illustrate the thermal conductivity (κ) of lead-based and tellurium-based chalcogenides at temperatures of 300, 600 and 800 K, within an energy range of -2 to 2 eV. Fig. 10 shows Thermal conductivity of a)PbO, b)PbS, c)PbSe, and d)PbTe bulk chalcogenides. Fig. 11 shows Thermal conductivity of a)SiTe, b)GeTe, c)PbTe, and d)SnTe bulk chalcogenides. In all samples, the thermal conductivity increases with increasing temperature. This can be attributed to the increased density and vibrations of the charge carriers (electrons and holes) and an increase in the speed of dispersion. Electrical conductivity happens between the charges due to the transfer of energy in the form of voltage or current,



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whereas thermal conductivity is the transfer of energy between the molecules due to the impact of pressure called heat. In conductive structures, these values are higher than semi-conductive structures.

To enhance the TE properties, materials should have a high Seebeck coefficient (S) and electrical conductivity (σ), while maintaining a low thermal conductivity. According to [72], the optimal temperature to achieve the lowest thermal conductivity is 300 K. As observed in the figure, when the charge carriers are electrons, the thermal conductivity is higher compared to when the carriers are holes. According to equation 1, the higher Seebeck coefficient and electrical conductivity, and lower thermal conductivity, it causes the amount of ZT in the material to increase. According to the obtained values, among the bulk's materials, PbTe has the maximum ZT and among the nanolayers, PbO has the highest ZT value. Therefore, PbTe bulk and PbO nanolayers show promising potential for thermoelectric applications.

**3.4. Optical properties:**

In this section, the optical properties of bulk chalcogenides, specifically XTe (X = Si, Ge, Sn and Pb) and PbY (Y =O, S, Se and Te), have been investigated using the GGA approximation and epsilon.x code. These optical properties are obtained from the dielectric function, which is a complex quantity that describes the linear response of the material to electromagnetic radiation. The dielectric function consists of two parts: the real part ($\varepsilon_1$) and the imaginary part ($\varepsilon_2$). The response of materials to light is shown by dielectric function. This function should have two real and imaginary parts. The real part of this function shows light emission and the imaginary part shows light absorption in the material. When the imaginary value of the dielectric function of a material is higher, it is a better absorber and it is used in optical applications related to absorbers. Materials with higher real part are also used in light emission applications.

The imaginary part of the dielectric function is calculated using the following formula from a theoretical perspective [73]:



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$$\varepsilon_2(\omega) = \frac{4\pi^2 e^2}{m^2\omega^2} \sum_{i,f} \int \frac{2dk^3}{(2\pi)^3}^2 |\langle ik|P_a|fk\rangle|^2 \times f_i^k(1-f_f^k)\delta(E_f^k - E_i^k - \omega) \quad (2)$$

The relation mentioned represents the contribution of transitions between bands. In this relation, |*ik*> represents the state vector of the initial position, |*fk*> represents the state vector of the final position, $f_i^k$ is the Fermi distribution function for occupied states, and $f_f^k$ is the Fermi distribution function for unoccupied states. The $\varepsilon_1$ can be calculated using the $\varepsilon_2$ and the Kramers-Kronig relation [74-76]:

$$\varepsilon_1(\omega) = \delta_{a\beta} + \frac{2}{\pi} Pr \int_0^\infty \frac{\omega' \, \mathrm{Im}[\varepsilon_{a\beta}(\omega')]}{\omega'^2 - \omega^2} d\omega' \quad (3)$$

Figures 12(a, b), and 13(a, b), display the real part ($\varepsilon_1$) and imaginary part ($\varepsilon_2$) of the dielectric function for bulk chalcogenides, specifically XTe (X = Si, Ge, Sn and Pb) and PbY (Y = O, S, Se and Te), as a function of energy. Fig. 12 shows the real part of the dielectric function for a) PbY (Y=O, S, Se and Te) and b) XTe (X=Si, Ge, Sn and Pb) bulk chalcogenides. Fig. 13 shows the imaginary part of the dielectric function for a) PbY (Y=O, S, Se and Te) and b) XTe (X=Si, Ge, Sn and Pb) bulk chalcogenides. From the $\varepsilon_2$ data, it is evident that certain chalcogenide compounds possess an optical gap. The optical gap values for PbTe, PbSe, PbS, and GeTe bulk materials are 0.8 eV, 1.8 eV, 2 eV and 0.1 eV, respectively. Also, the optical gap of PbTe, PbSe, PbS, and GeTe nanolayers is 0.76, 1.5, 1.85 and 0.05 eV, respectively. The decrease in the optical gap of nanolayers compared to bulk indicates that electrons need less energy to be excited and create a phase transition in the nanolayer structure.

Figure 13 reveals that $\varepsilon_2$ becomes zero for PbO and PbTe materials at energies higher than 8 eV and for GeTe composition at energies higher than 4 eV. Additionally, the $\varepsilon_2$ values for PbS, PbSe and SnTe chalcogenides become zero at energies higher than 5 eV and for the SiTe compound at energies higher than 7 eV. In these energy ranges, these materials are not transparent; instead, they appear dark and do not allow penetration of electromagnetic waves. Consequently, they can be utilized as absorbent materials [77].



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In the energy range of 0 to 4 eV, the $\varepsilon_2$ exhibits an initial increase followed by a decrease. This behavior indicates the occurrence of inter-band transitions in these compounds. Figure 12 reveals that the $\varepsilon_1$ is negative in the range of 2 to 5 eV, indicating that waves do not propagate in this energy region. The surfaces of these compounds can be utilized as magnetic filters to absorb waves within this energy range. Furthermore, the static dielectric constant ($\varepsilon_1$ at zero energy) for PbTe, PbSe, PbS, GeTe, and SnTe compounds is approximately 20, 18, 17, 79, and 43, respectively. The static refractive index ($n_0$) of these materials can be obtained by taking the square root of the static dielectric constant. Specifically, the values of $n_0$ are 4.47, 4.24, 4.12, 8.88, and 6.55 for PbTe, PbSe, PbS, GeTe, and SnTe bulk chalcogenides, respectively. The refractive index values for PbTe, PbSe, PbS, GeTe, and SnTe nanolayers are 1.58, 1.51, 1.54, 2.23, and 1.87, respectively. The decrease in the refractive index of nanolayers compared to bulks indicates more absorption of light by nanolayers.

Table 4 presents the optical gap and $n_0$ values from this study as well as other research works. To calculate the reflectivity (R) and absorption coefficient (A), the following relations are employed:

$$R = \left| \frac{(n(\omega)-1)^2 + k(\omega)^2}{(n(\omega)+1)^2 + k(\omega)^2} \right| \tag{4}$$

$$A(\omega) = \frac{2k(\omega)E}{\hbar c} \tag{5}$$

In the given formula, n and k represent the real and imaginary parts of the refractive index (or optical coefficients). These coefficients can be expressed in terms of the real and imaginary parts of the dielectric function as follows:

$$n(\omega) = \sqrt{1/2\left\{\sqrt{(\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2)} + \varepsilon_1(\omega)\right\}} \tag{6}$$



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$$k(\omega) = \sqrt{1/2\left\{\sqrt{(\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2)} - \varepsilon_1(\omega)\right\}} \quad (7)$$

When light is applied to a material, part of it is absorbed, another part is transmitted and the final part is reflected. The resistance of a material to the transmitted of light is called optical resistance. Figures 14(a, b), and 15(a, b) depict the graphs of the absorption and reflectance coefficients as a function of energy for these materials, considering the vertical direction of the electric field. Fig. 14 shows the optical absorption of a) PbY (Y=O, S, Se, and Te) and b) XTe (X=Si, Ge, Sn, and Pb) bulk chalcogenides. Fig. 15 shows the optical reflectivity of a) PbY (Y=O, S, Se, and Te) and b) XTe (X=Si, Ge, Sn, and Pb) bulk chalcogenides. Upon careful examination of these figures, it is evident that the reflection is minimal at low energies and the variations in these functions exhibit a direct relationship with changes in energy. Optical Absorption Edge' refers to the photon energy level at which the absorption behavior of semiconductors changes, characterized by an optical gap. It can be analyzed using the Tauc formula above the optical gap and the Urbach formula below it. A higher absorption edge in a material corresponds to a larger optical gap, indicating improved absorption properties in the visible region. The findings of this study reveal that PbS exhibits the largest optical gap among nanolayers, while GeTe shows the largest optical gap in bulk form.

**4. Conclusions**

In this article, the electronic, structural, thermoelectric and optical properties of bulk and nanolayers chalcogenides, XTe (X = Si, Ge, Sn, and Pb) and PbY (Y = O, S, Se, and Te) were investigated using the DFT and the semiclassical Boltzmann method. The calculations conducted in this research demonstrated that these materials exhibit significant potential in thermoelectric applications, primarily due to their high S and σ coefficients. The electronic band structure analysis revealed that PbO, PbS, PbSe, PbTe, and



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GeTe compounds are direct band-gap semiconductors. Additionally, the valence bands of SiTe and SnTe compounds slightly intersect the Fermi energy level, indicating the metallic nature of this particular group of materials. In the nanolayer structure, the energy gap was changed, the GeTe material changed from a semiconductor to a metal. The PbTe compound exhibits the highest Seebeck coefficient at 300 K, indicating its superior thermoelectric properties compared to other materials in this group. Also, the thermoelectric properties of some materials in the nanolayer state were significantly improved. The most promising potential for thermoelectric applications is PbTe bulk and PbO nanolayer. Furthermore, the optical analysis revealed that the imaginary part of the dielectric function ($\varepsilon_2$) initially increases and then decreases in the energy range of 0-4 eV, indicating the occurrence of inter-band transitions in these compounds. PbS material has the lowest refractive index and the highest optical gap in both the bulk and the nanolayer structure, making it a suitable option for optoelectronic applications.

**Data Availability Statement:**

No Data associated in the manuscript.

**Acknowledgment:**

The computing resources utilized in this research were supported by the Dena High-Performance Computing (HPC) facility at Yasouj University.

**Conflict of interest:**

The authors declare that they have no conflict of interest.

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## Figures captions:

**Fig. 1.** Pb/Te-based chalcogenides structure. a) primitive unit cell, b) conventional unit cell.



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**Table 1.** Calculated equilibrium lattice constant a (Å) and coherence energy (eV).

| chalcogenides | a (Å) | coherence energy(eV) | a (Å) others |
|---|---|---|---|
| SiTe | 5.843 | 13.43 | - |



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| | | | |
|---|---|---|---|
| GeTe | 6.024 | 13.75 | 5.95 [78] |
| SnTe | 6.389 | 12.95 | 6.31 [79] |
| PbTe | 6.574 | 13.06 | 6.46 [80] |
| PbSe | 6.229 | 5.61 | 6.124 [81] |
| PbS | 6.009 | 6.65 | 5.923 [82] |
| PbO | 5.265 | 8.47 | 5.51 [83] |

**Table 2.** Structural parameter of bulk Pb/Te-based chalcogenides.

| Primitive cell | | Conventional cell | |
|---|---|---|---|
| Δ 1-2-3=60° | 1-2=4.26 Å | Δ 7-8-10=90° | 9-11=3.012 Å |
| Δ 1-2-6=90° | 1-3=4.26 Å | Δ 8-7-9=90° | 10-11=3.012 Å |
| Δ 2-6-3=90° | 2-6=3.012 Å | 7-8=3.012 Å | 7-10=5.2174 Å |
| Δ 3-4-5=120° | 1-6=5.217 Å | 7-11=4.26 Å | 9-10=4.26 Å |
| Δ 3-6-4=90° | 6-4=3.012 Å | | |

**Tables 3.** Seebeck coefficient and band gap energy of Pb/Te-based chalcogenides.

| Materials (bulk and nanolayers [57]) | S (μV/κ) | $E_g$ (eV) |
|---|---|---|
| PbO bulk-PbO nanolayer | 574-2161 | 0.17-1.367 |



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| | | |
|---|---|---|
| PbS bulk-Pbs nanolayer | 915-1130 | 0.75-0.706 |
| PbSe bulk-PbSe nanolayer | 842-859 | 0.57-0.509 |
| PbTe bulk-PbTe nanolayer | 1527-424 | 0.85-0.257 |
| SiTe bulk-SiTe nanolayer | 107-33 | metal-metal |
| GeTe bulk-GeTe nanolayer | 763-634 | 0.5-metal |
| SnTe bulk-SnTe nanolayer | 233-80 | metal-metal |

**Table 4.** The optical gap and $n_0$ of Pb/Te-based chalcogenides.

| Materials | $n_0$ | Optical gap (eV) | Other works |
|---|---|---|---|
| PbTe | 4.47 | 0.8 | 5.5-0.81 [84] |
| PbSe | 4.24 | 1.8 | 4.25-1.5 [85] |
| PbS | 4.12 | 2.0 | 4.1-1.8 [85] |
| Gete | 8.88 | 0.1 | 6.2-0.07 [86] |
| SnTe | 6.55 | 0.01 | 6.4-0.03 [86] |



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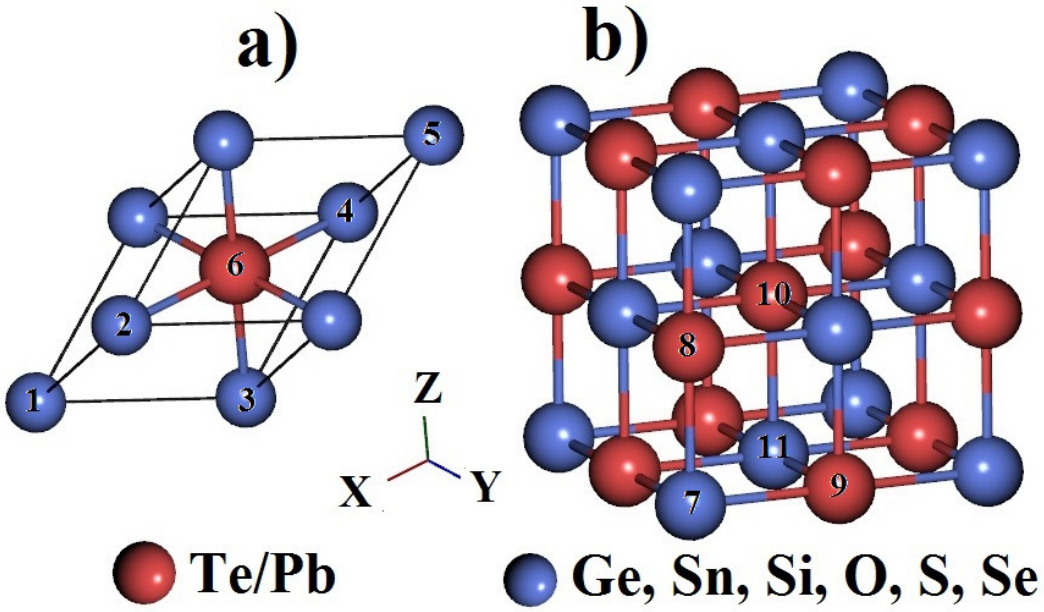


**Fig. 1.**

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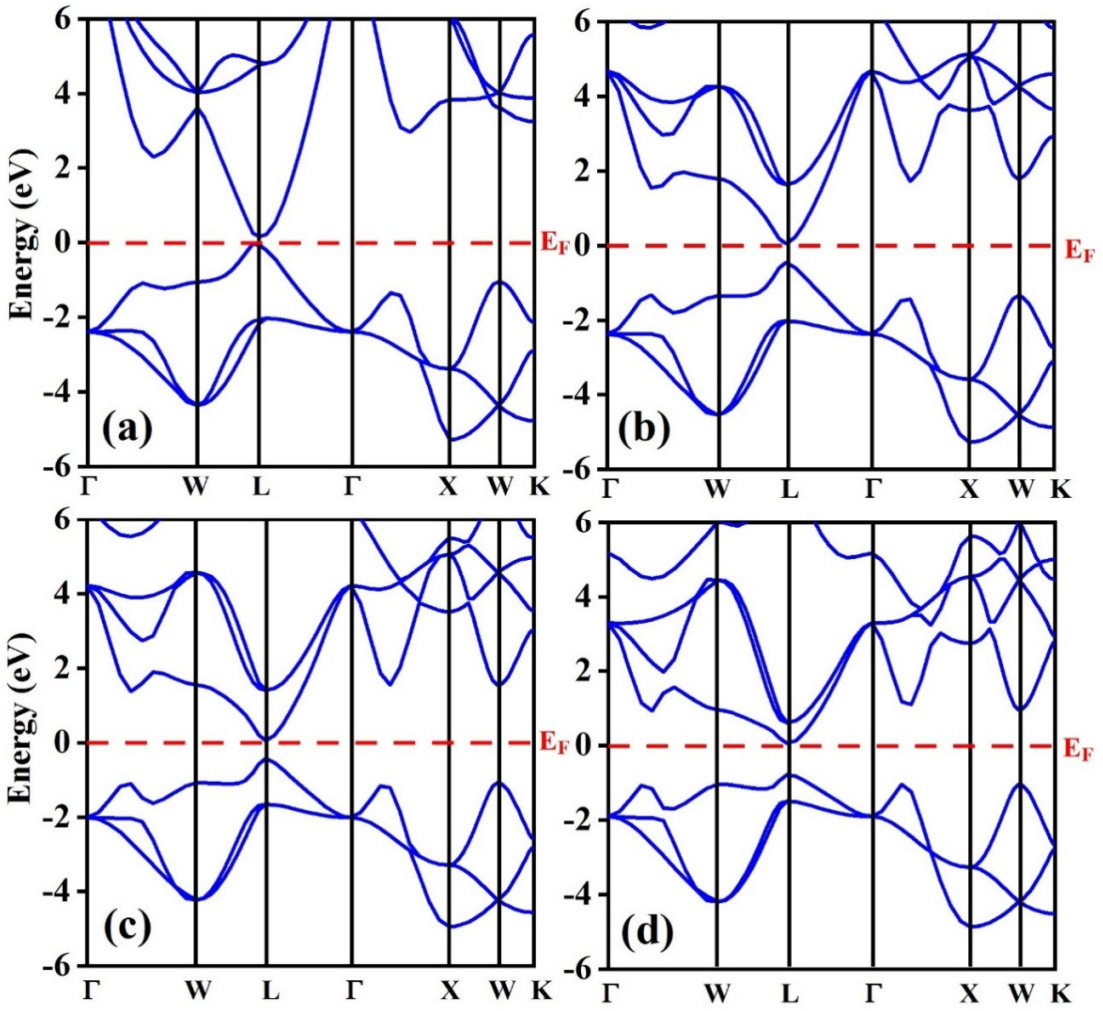


**Fig. 2.**

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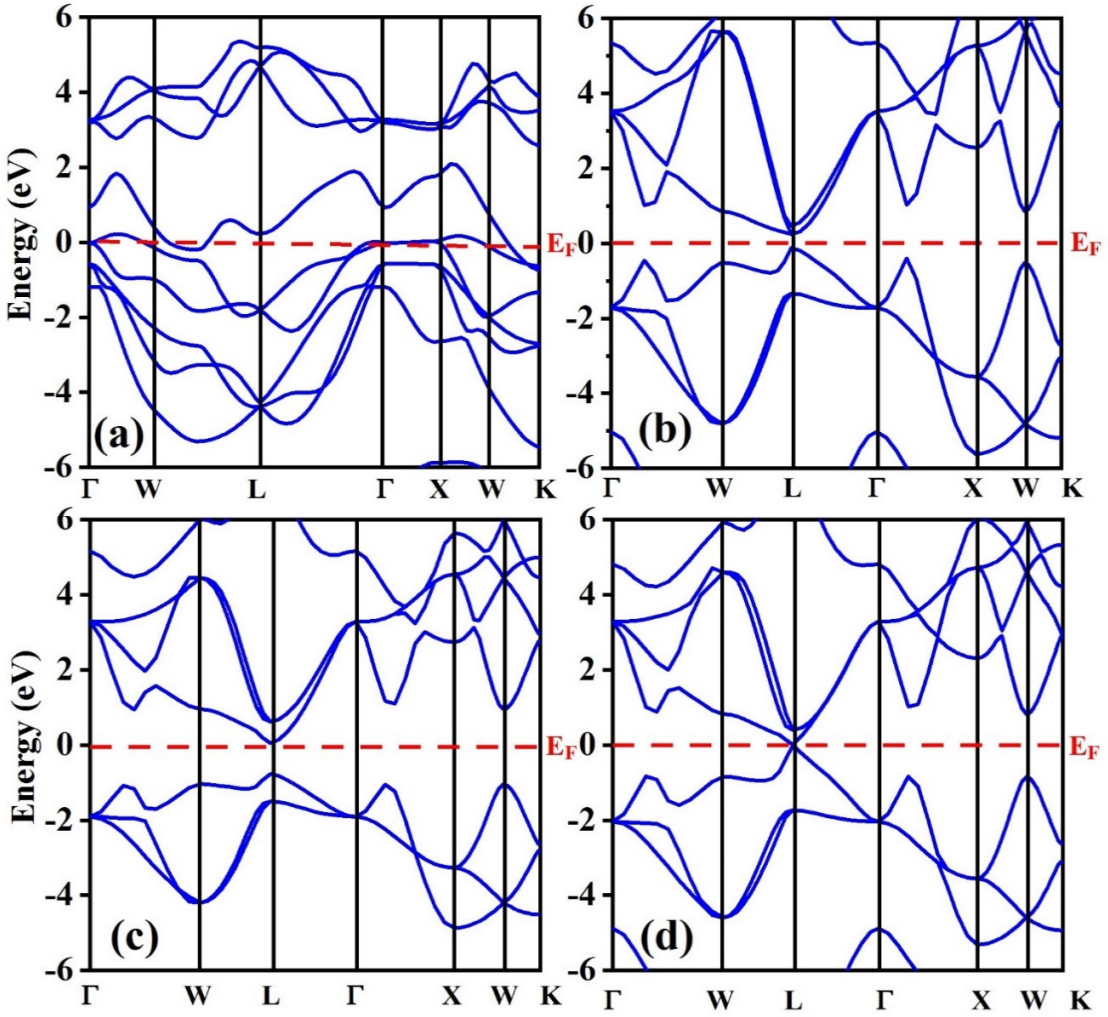


**Fig. 3.**

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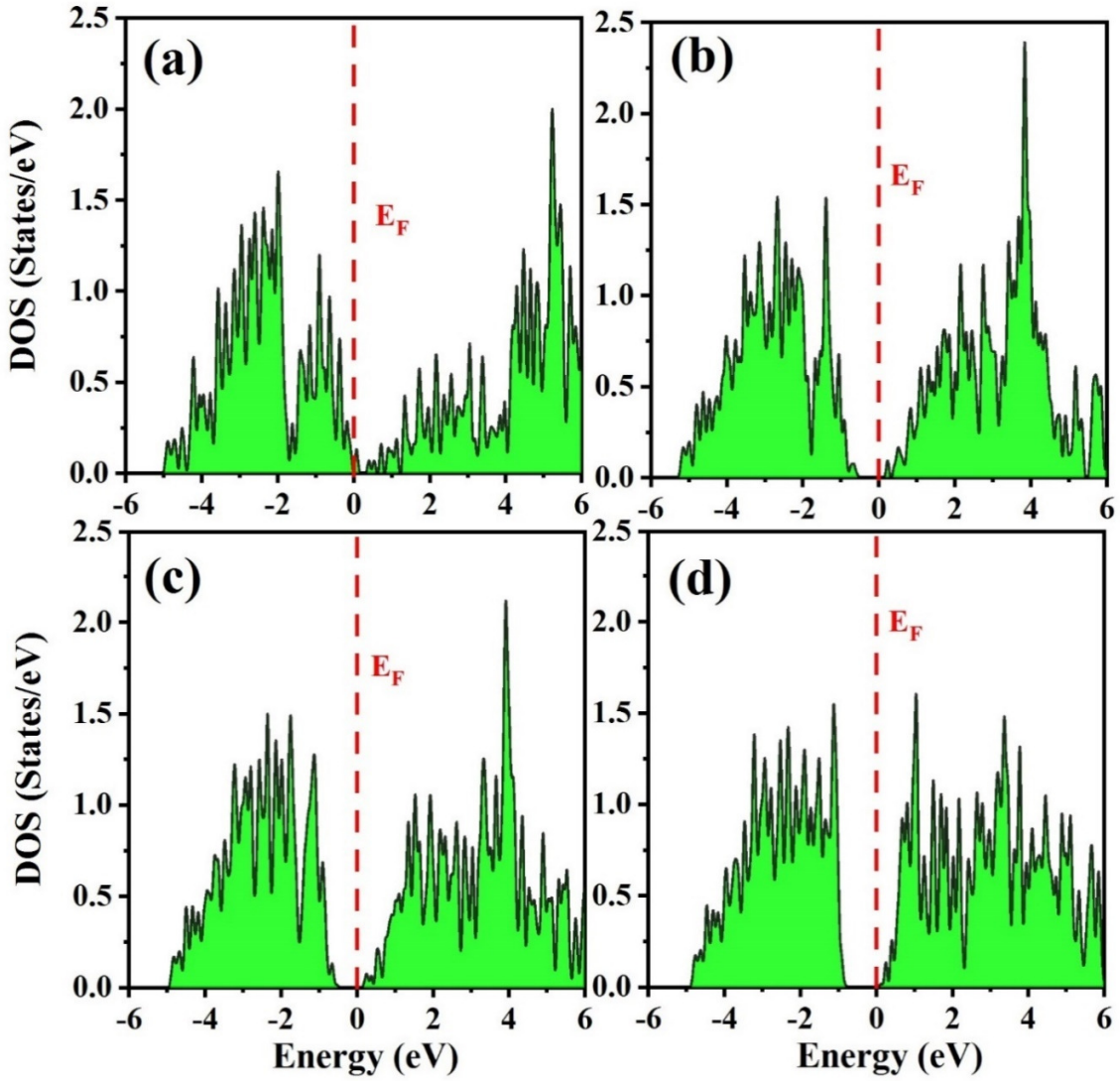


**Fig. 4.**

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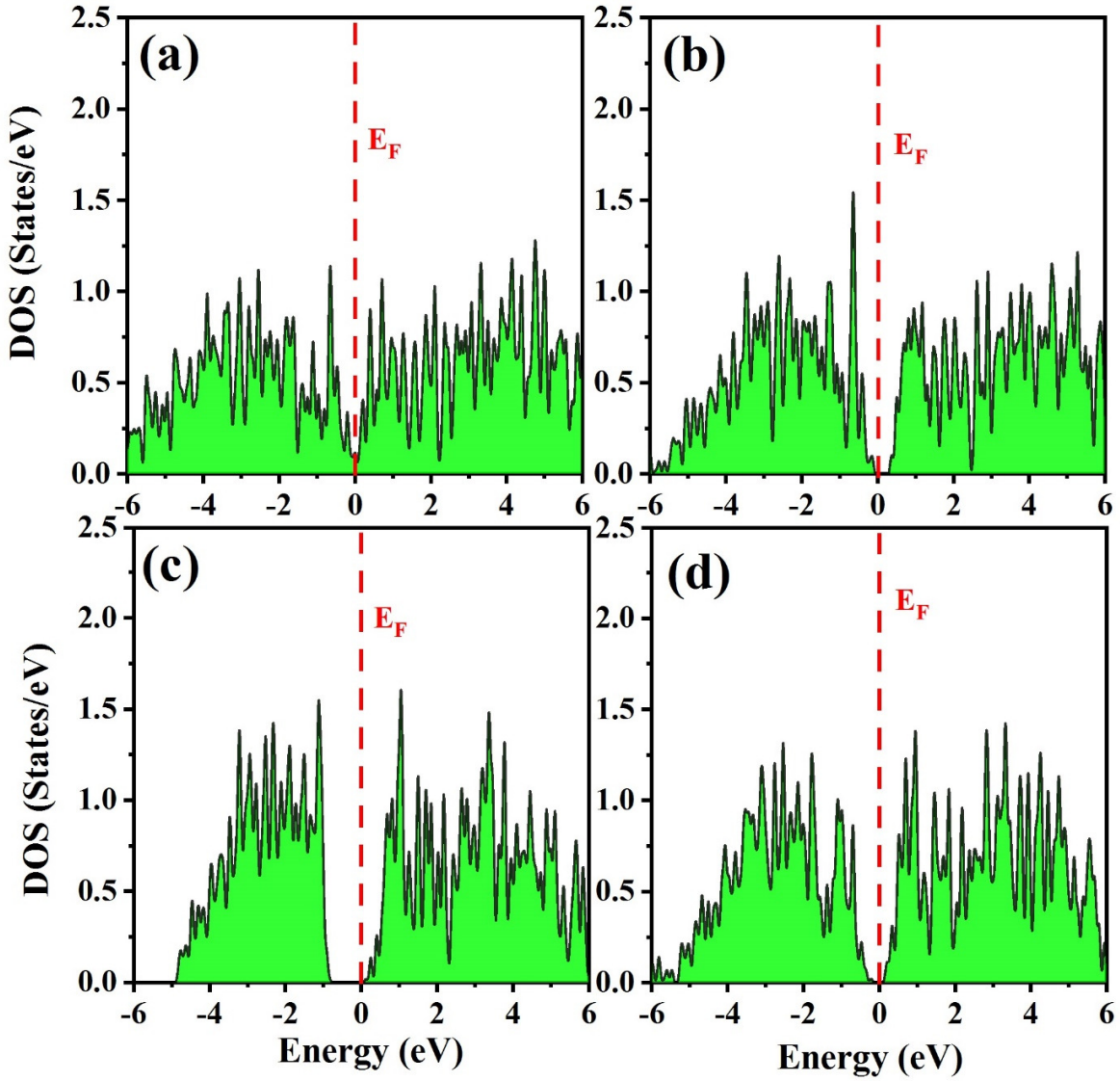


**Fig 5.**

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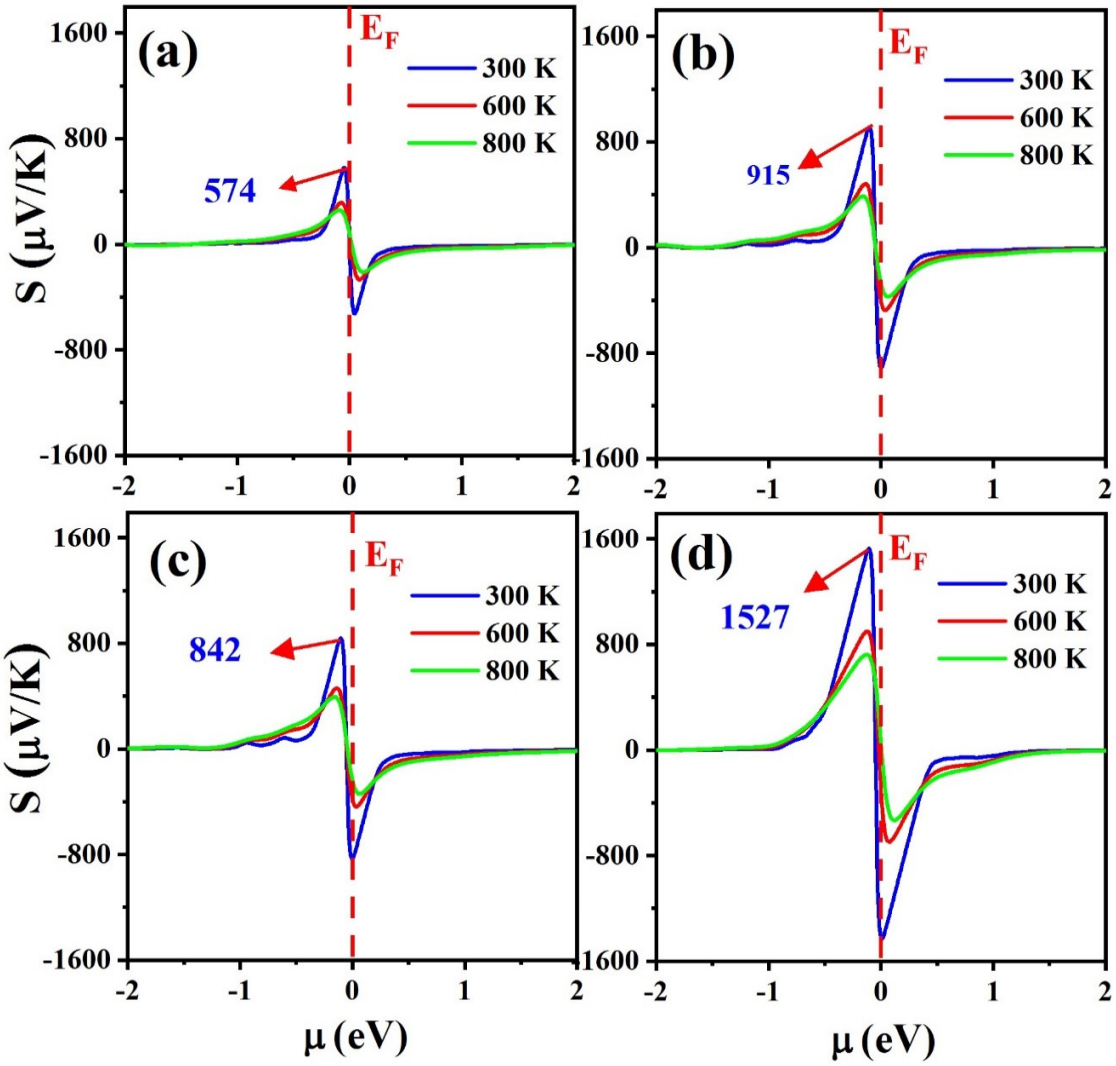


**Fig 6.**

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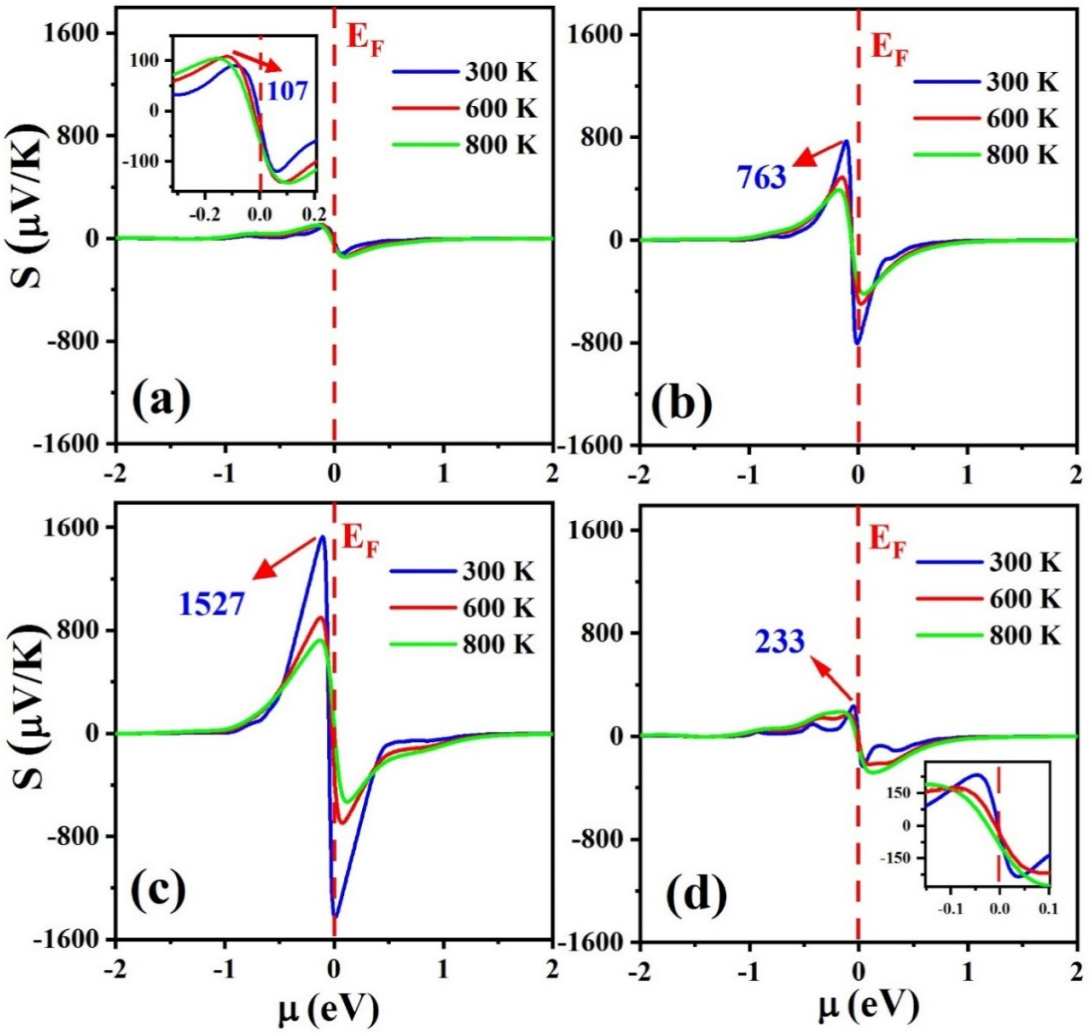


**Fig 7.**

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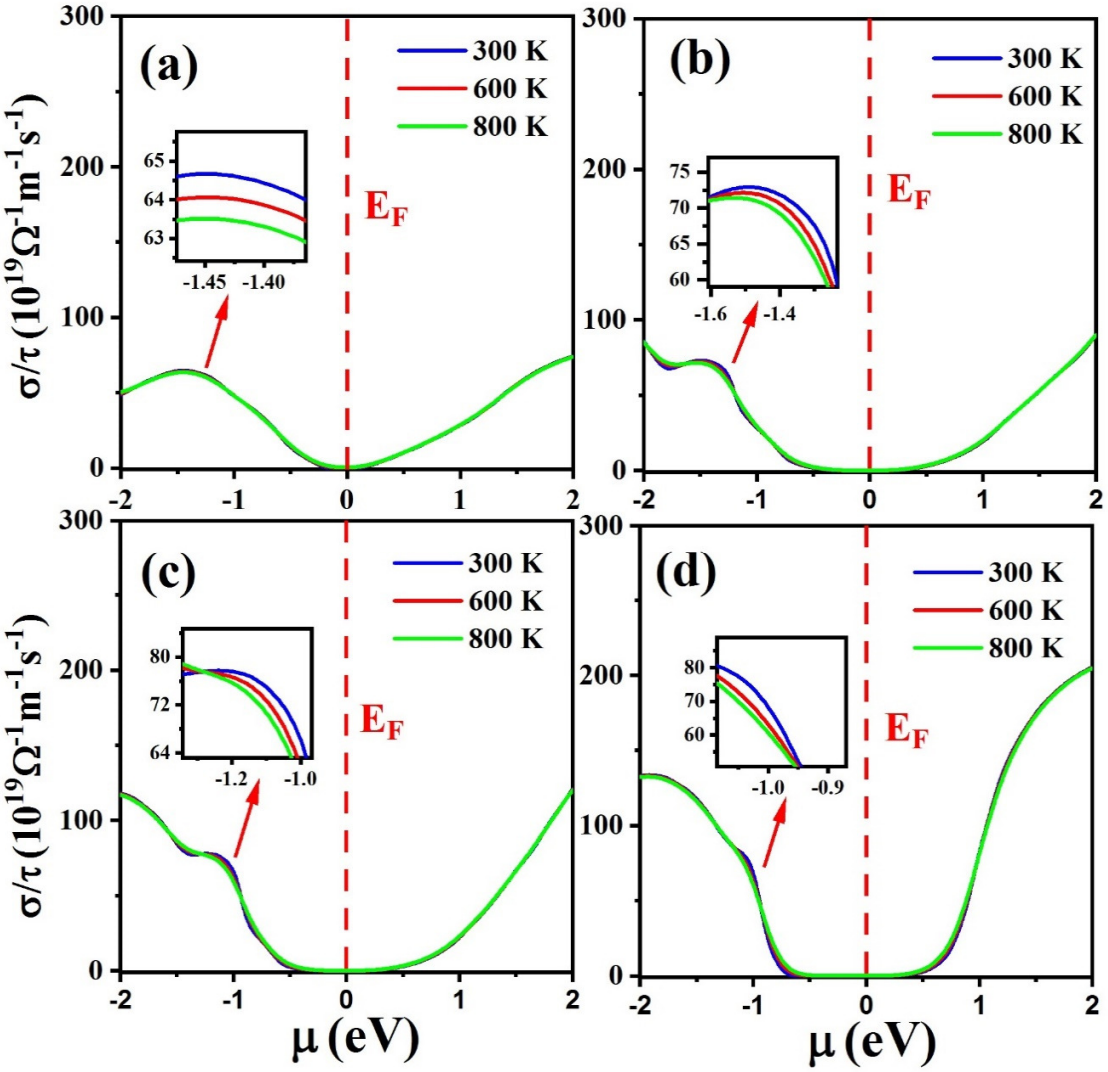


**Fig. 8.**

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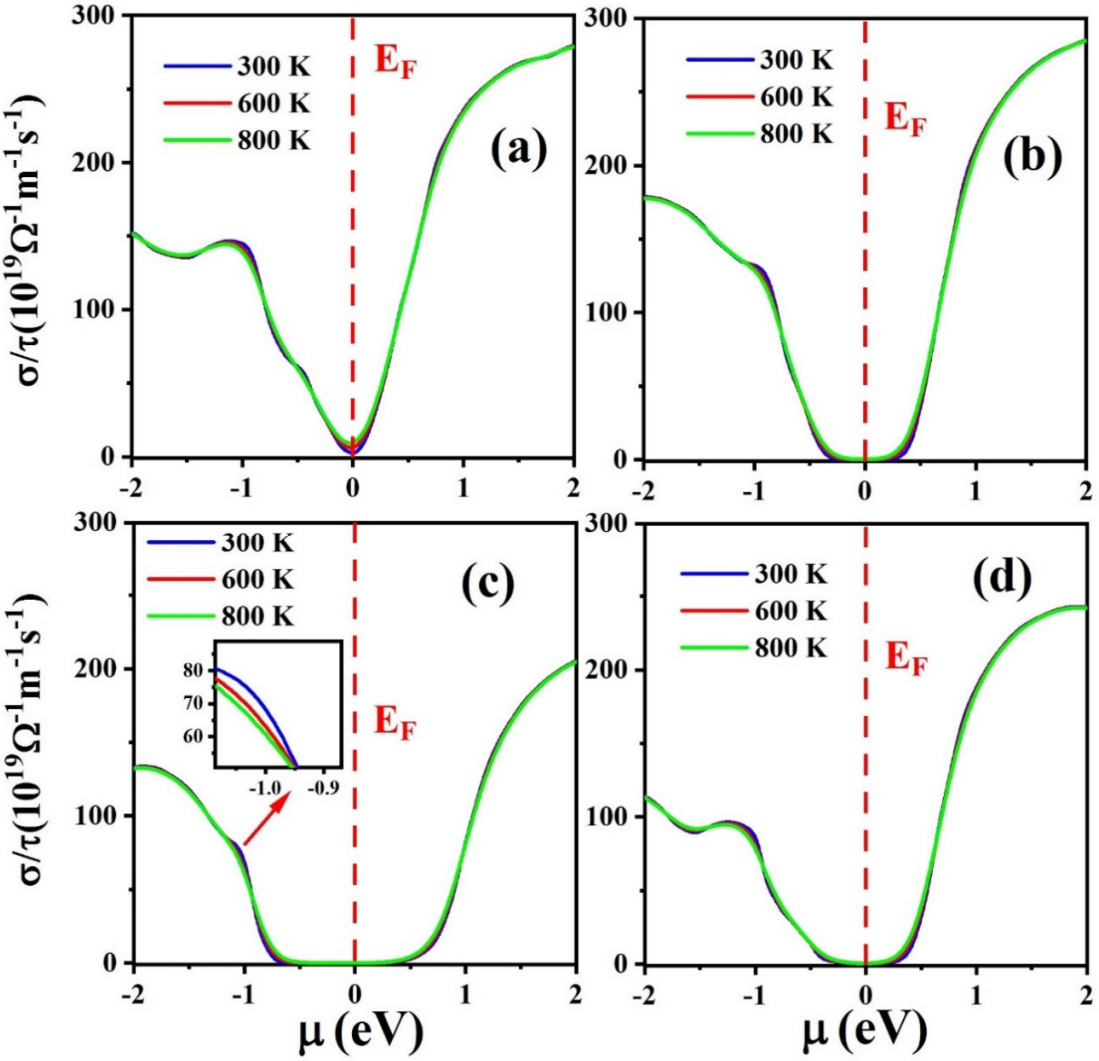


**Fig. 9.**



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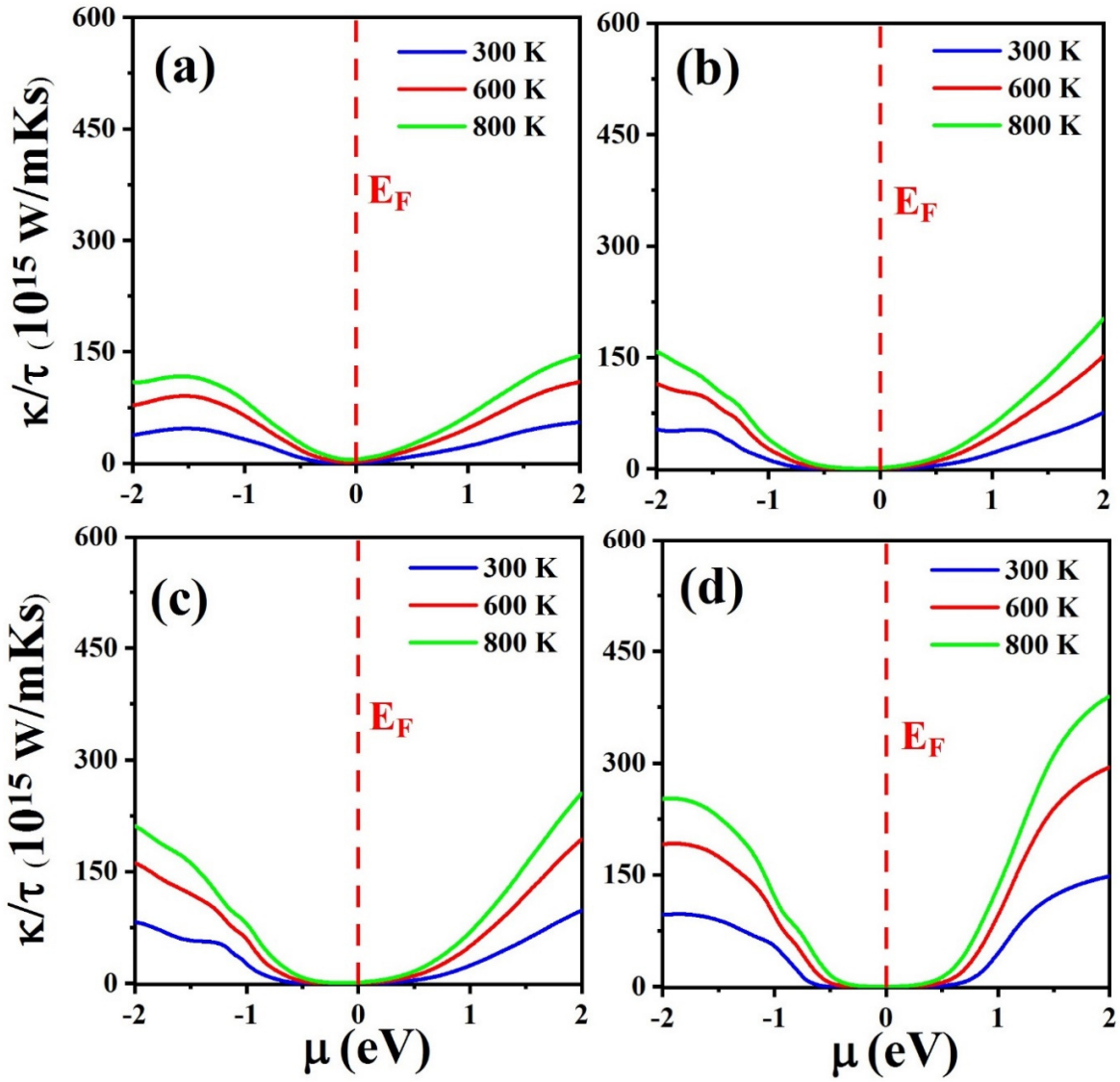


**Fig. 10.**

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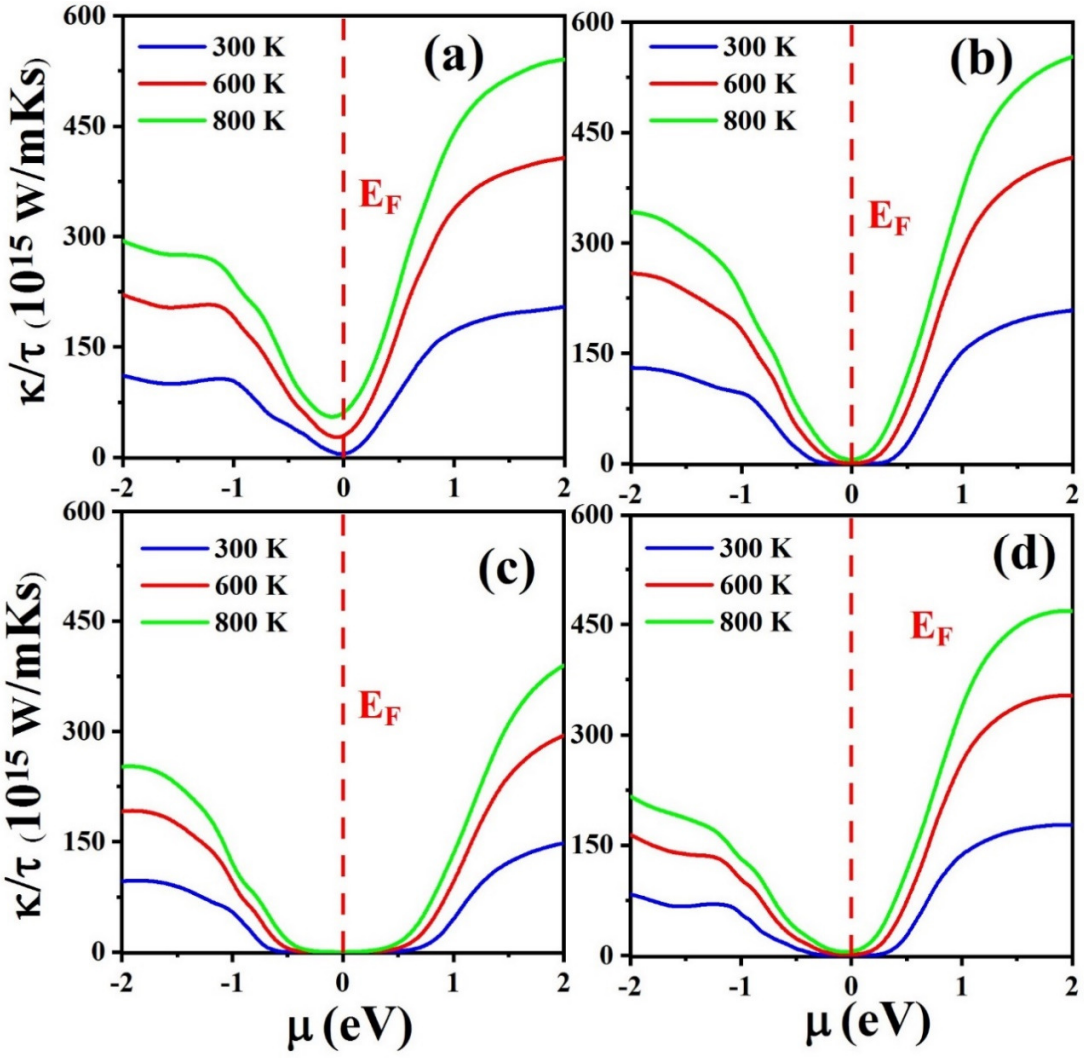


**Fig. 11.**

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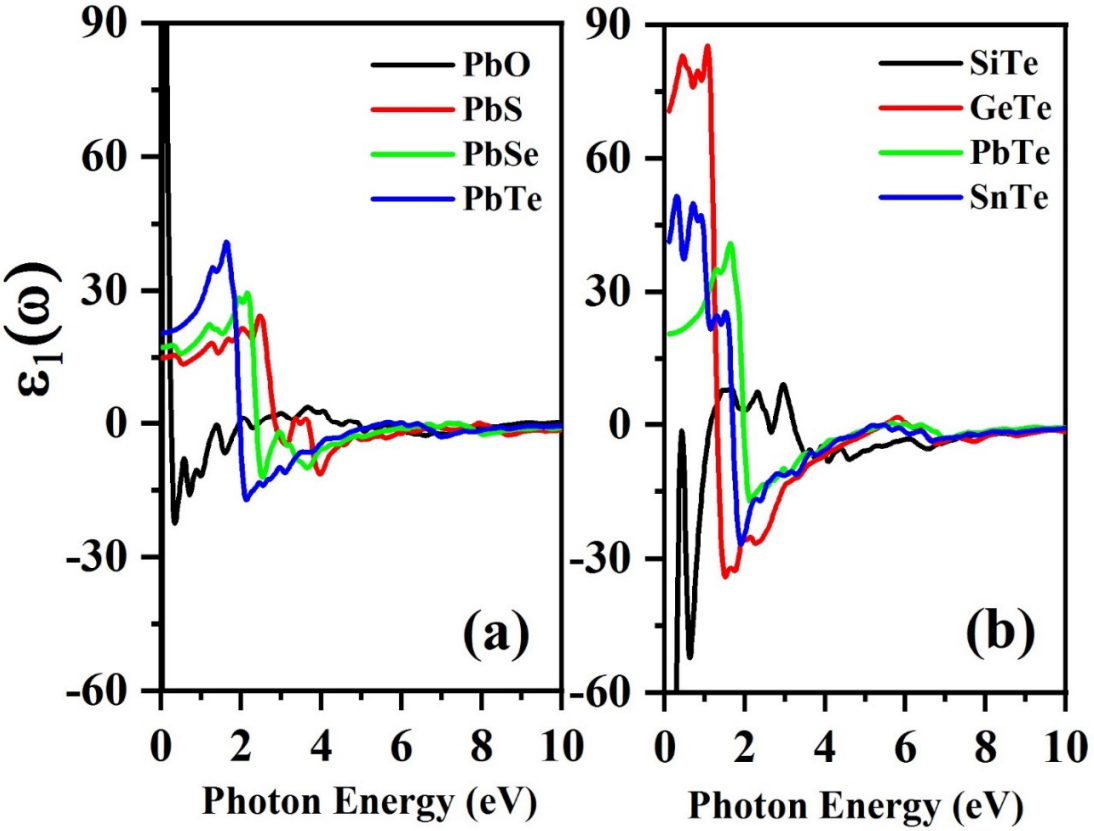


**Fig. 12.**

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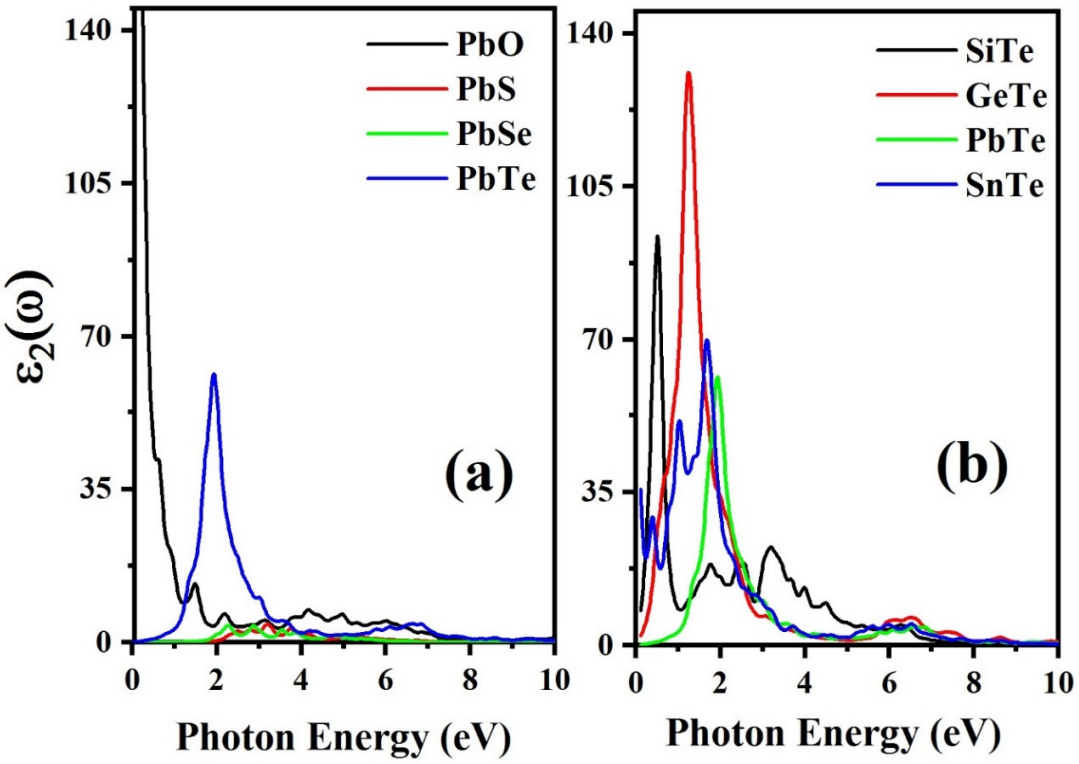


**Fig. 13.**

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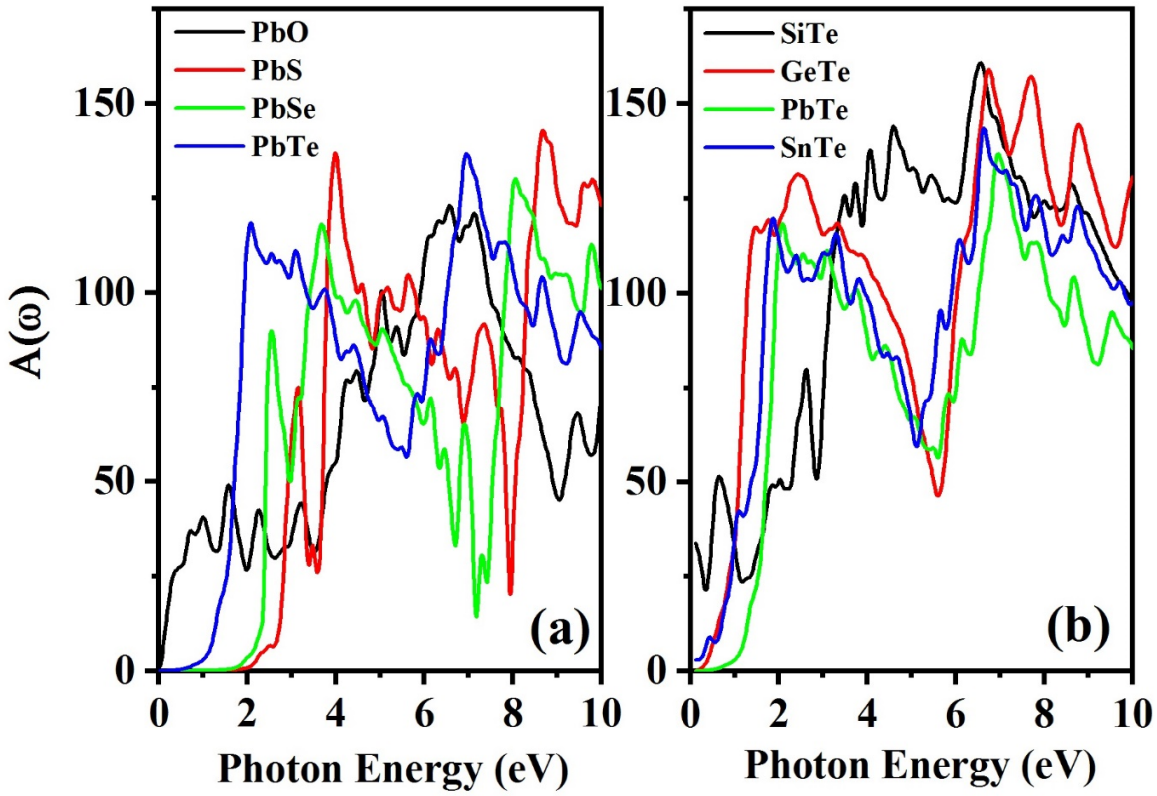


**Fig. 14.**

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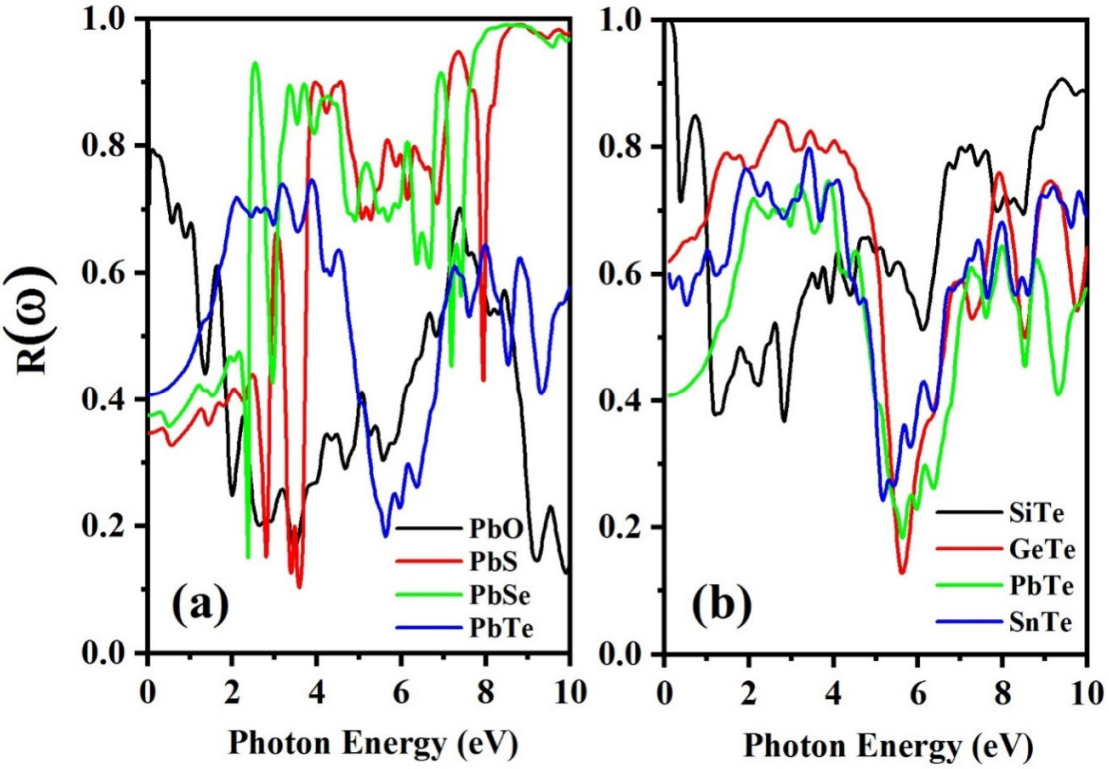


**Fig. 15.**



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