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THE INFLUENCE OF PRESSURE ON THE LATTICE CONSTANT IN THE BINARY COMPOUND VTE IN THE ZENC BLEND CASE

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Abstract:

The structural, electronic, and optical characteristics of the (ZB) VTe bulk are investigated using first-principles simulations based on density functional theory (DFT). The magnitude of the lattice constant when the pressure was zero was 8.54 Å and the amount of the energy gap was 1.19 eV, but after applying a pressure of 15 kPa, the lattice constant will decrease to 7.2 Å While the energy gap increases to 1.5 eV. In general, pressure decreases the lattice constant in solids. This is because pressure pushes the atoms closer together, reducing the amount of space between them. The lattice constant is the distance between adjacent atoms in a crystal, so a decrease in the lattice constant means that the crystal is being compressed. The effect of pressure on the lattice constant is not uniform for all solids. Some solids are more compressible than others, meaning that they will decrease in volume more significantly under pressure. The compressibility of a solid depends on a number of factors, including the type of bonds between them.

Keywords: VTe; pressure; bulk properties; DFT; optical characteristics;

INTRODUCTION

The effect of pressure on the lattice constant in materials is considered an important aspect in studying the properties of materials and their behavior under different conditions. The lattice constant refers to the distance between lattice points in a material, and a change in this constant can greatly affect the properties of the material. When a material is subjected to pressure, it is affected by forces that change its shape and size. When the stress on the material increases, the mesh points move closer together, causing the mesh constant to decrease. Conversely, when the stress on the material decreases, the lattice points move away from each other, causing the lattice constant to increase. The effect of material pressure on the lattice constant in turn affects the mechanical properties of the material [1,2]. For example, in solid materials, the lattice constant is a determinant of the hardness of the material. When the lattice constant decreases, the bonds between the molecules of the material become stronger, increasing its rigidity. Conversely, when the lattice constant increases, the bonds between the material molecules become weaker, reducing their stiffness. In addition, the pressure of a material affects its thermal properties [3-5]. When the lattice constant decreases, temperature changes lead to smaller changes in the volume of the material. Conversely, when the lattice constant increases, temperature changes lead to larger changes in the volume of the material. Also, the pressure of a material can affects its electrical and magnetic properties. For example, in semiconductor materials, increasing pressure can increase the conductivity of the material, while decreasing pressure can decrease the conductivity of the material. In general, it can be said that the effect of pressure on the lattice constant in materials depends on the type of material and its atomic and molecular structure. Thus, studying this effect contributes to a better understanding of the behavior of materials under different conditions and the development of new applications [6].

Computational methods

This work computed the optical, magnetic, electric, phonon transport, and structural features of a (ZB) VTe bulk using density functional theory and the CASTEP technique [7]. These features include optical, magnetic, electric. Generalized gradient approximations (GGA) and the PBE technique have been used to analyses the exchange-correlation energy [8]. In order to remove any potential atom-atom interactions, the constructed system is a (ZB) VTe bulk with 15 Å inserted in a direction perpendicular to it. The constructed system is a (ZB) VTe bulk consisting of (15 × 15 × 15) per unit cell. The cutoff energy of 400 eV is used when examining plane waves. Every structure has attained its most relaxed state. The size of the atomic force is less than 0.01 eV/Å, but the magnitude of the total energy affinity is 10^{-6} eV.

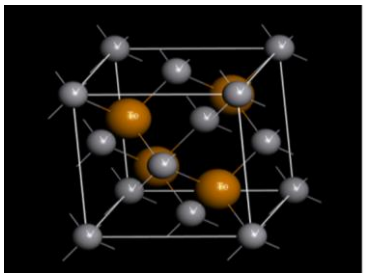


Fig. 1.Crystal structure of (RS) VTe bulk

RESULTS AND DISCUSSION

3.1 Electronic structures of (ZB) VTe bulk

In Figure 2, when a pressure of 15 GPa is applied, the energy gap will increase due to the small lattice constant of this compound, as shown in the energy band and density of states.

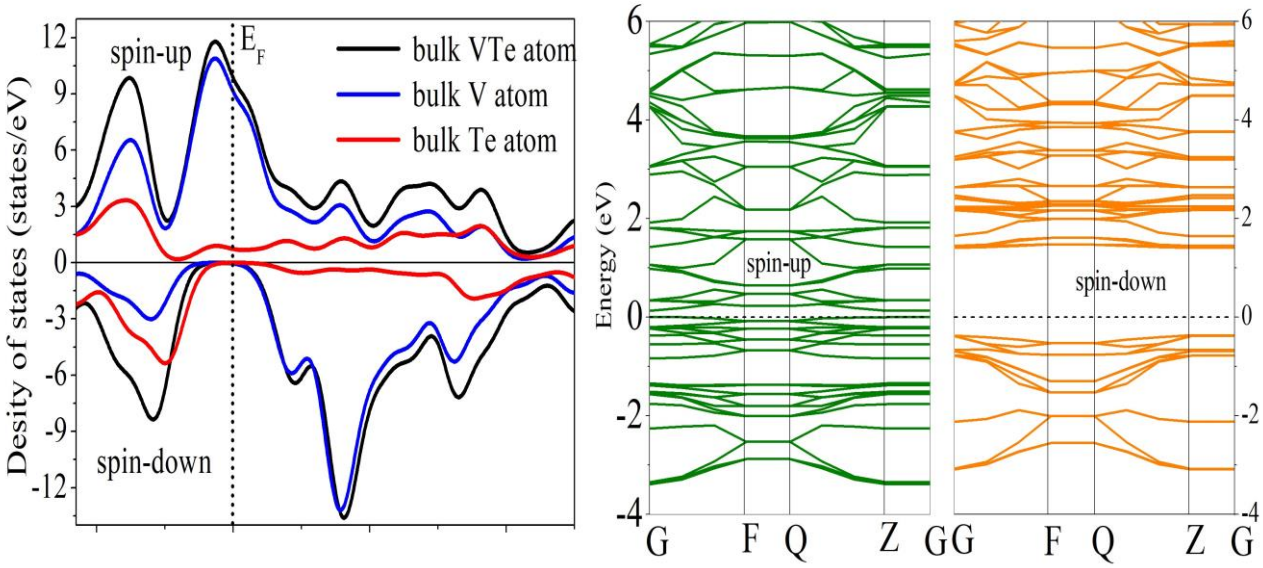


Fig. 2. The densities of states in the bulk 9ZB) VTe (right) and the band structure (spin up and spin down) of VTe (left) by effected 15 GPa

3.2 phonon transport

The necessity for a more thorough scientific knowledge of heat transmission through materials has been brought to light by recent advancements in the research of partly metallic materials. Density functional theory (DFT) simulations of first-principles calculations are a valuable technique for determining the scattering of phonons in the (ZB) VTe. Materials physics must include the study of phonons. In reality, phonons are essential for generating a wide range of physical characteristics, such as thermal conductivity and electrical conductivity A phonon is, in other words, the lowest quantity of energy that can be transmitted from an auditory source to a physical medium. In this case, the phonon is analogous to an electromagnetic wave isotope, or the lowest quantity of electromagnetic energy that can be transmitted from an electromagnetic wave to a physical medium [9]. The phonon dispersions of the (ZB) VTe monolayer are shown in Figure 3. Because the phonon dispersions do not have the imaginary vibrational frequency throughout the Brillouin region, the monolayer is dynamically stable.

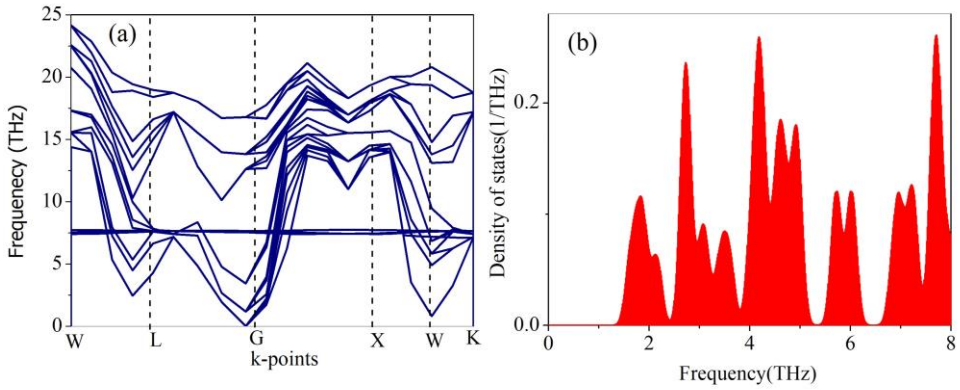


Fig. 3. Curves showing state density and phonon dispersion for bulk (ZB) VTe.

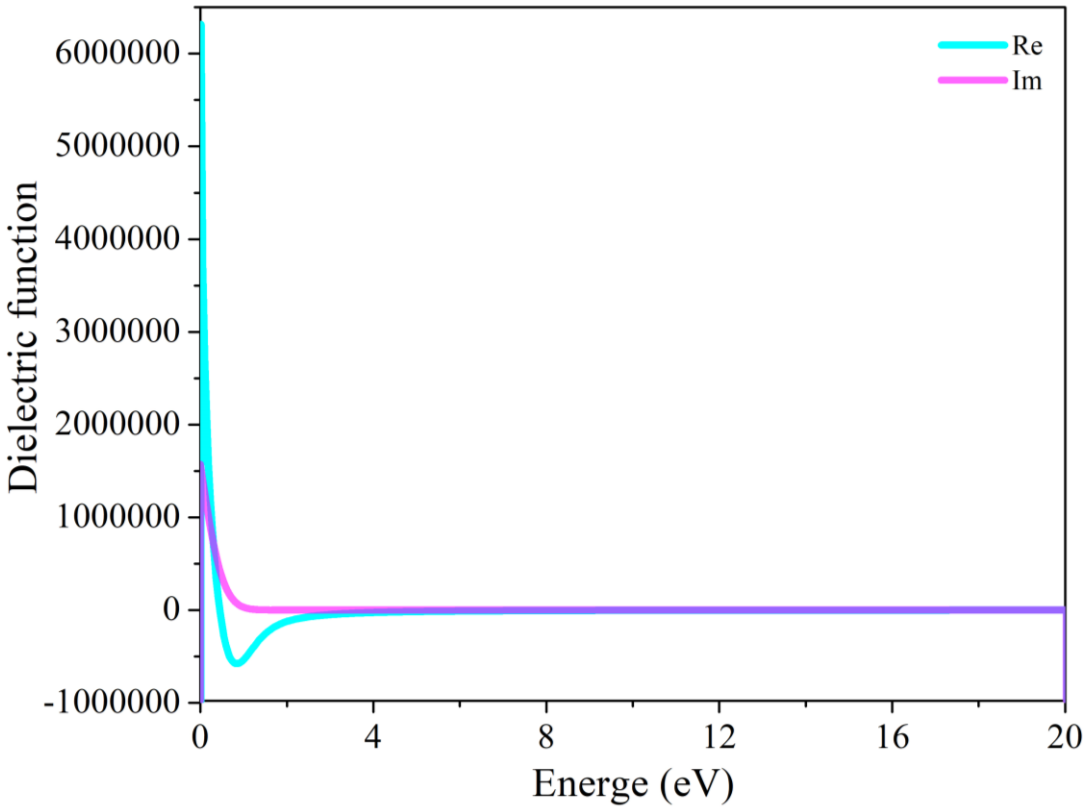
3.3 Optical Properties

The optical characteristics of materials are important for both basic science and contemporary applications. We computed the conductivity, dielectric function, loss function, refractive index, propagation constant (K), and absorption coefficient, among other optical parameters. Using the connection shown below, it can be concluded.

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

where the imaginary and real components of the dielectric function are represented by the $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, respectively. The electromagnetic field's propagative conduct has a connection to reality $\varepsilon_1(\omega)$ [10]. The Fermi golden rule is used for adding the occupied–unoccupied transitions to obtain the relationship for the imaginary part $\varepsilon_2(\omega)$ [11]. Figure 4 depicts the real and imaginary parts of the dielectric function. The (ZB) VTe has a dielectric function (at zero energy) of is 15×10^5 and 65×10^5. Furthermore, the non-negative real dielectric function indicates that the (ZB) VTe operates in the same manner as a semiconductor in this frequency range. UV radiation rapidly decreases with an increase in photon energy, but the insulation curve in visible areas expands and decreases with energy. It is generally known that materials that function effectively in visible and infrared light have gaps less than 1.8 eV. Consequently, the (ZB) VTe will operate as a visible and infrared visual material [12].

Fig. 4. Real and imaginary parts of the (ZB) VTe bulk dielectric function



The optical properties were studied in the energy range 0–20 eV. Figure 5 shows that absorption starts at energies lower than 0.07 eV in the infrared (IR) region and 1.3 eV for the (ZB) VTe. The existence of an IR absorption peak between (0.8 eV and 1.3 eV) was confirmed by our results. The absorption coefficient clearly indicates that the UV (8

eV) area is where its biggest peaks are located. Visible light absorption, which begins in the range of (1.5 eV and 3 eV), is one of the most important research areas on light absorption that may be used in the creation of solar cells. Another observation is the high UV light absorption energy of a single layer of (ZB) VTe, which might be used in photoelectronic devices such as UV detectors.

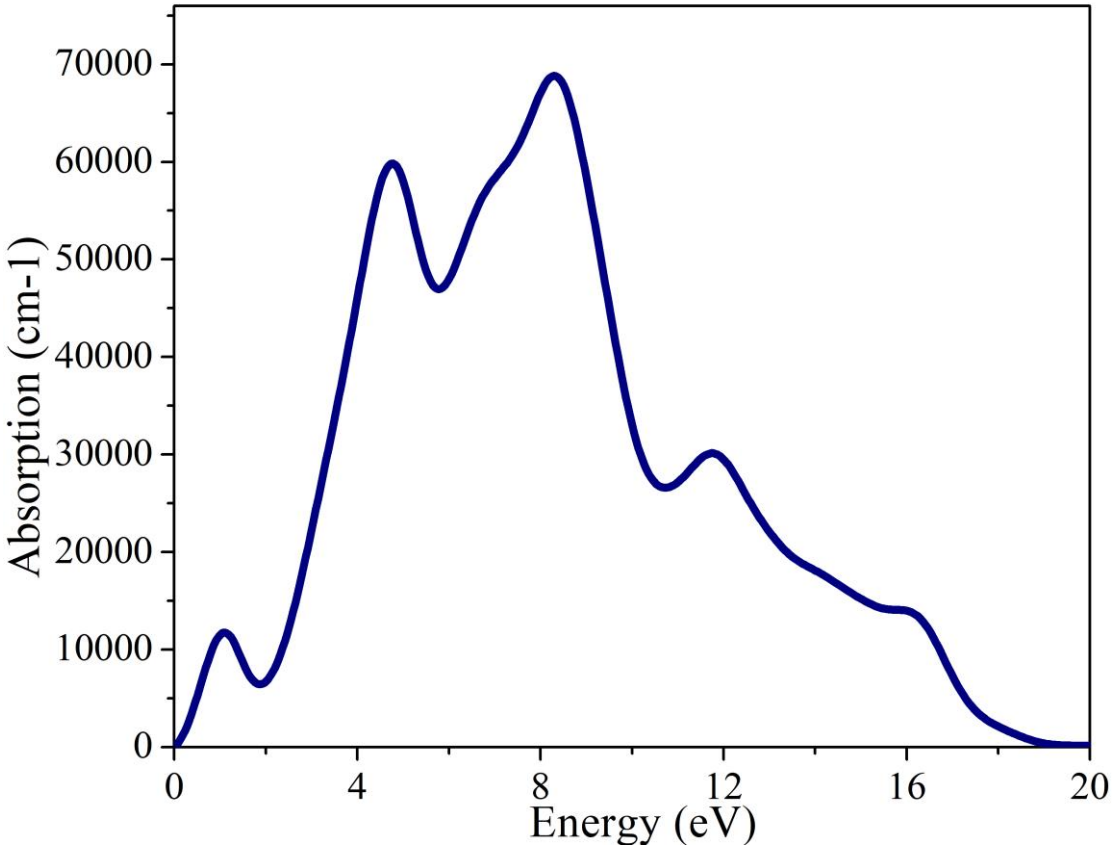


Figure 5: Optical absorption of (ZB) VTe bulk

The refractive index and propagation constant of the (ZB) VTe are shown vs photon energy in Figure (6). The (ZB) VTe monolayer has a refractive index of 1.9 and a propagation coefficient (at zero energy) of 7.9. Conversely, at 2.5 eV, the propagation constant reaches its maximum value of 2.9. The refractive index finally begins to decrease with energy at high photon energies, while it tends to decrease with energy in the visible spectrum and with UV radiation. The infrared area is often where the bulk has the maximum refractive index. For the photon, the spectra of the refractive index (n) and propagation constant (K) decrease rapidly and stabilize at 20 eV.

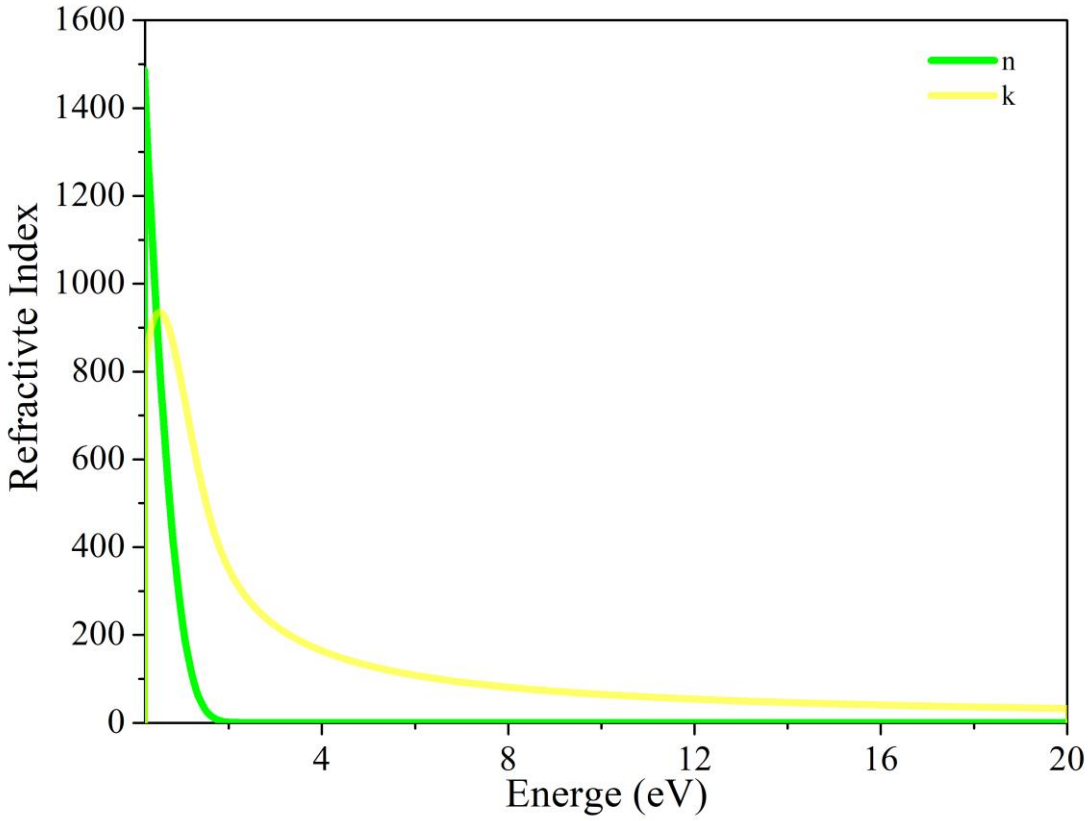


Figure 6: Refractive index and propagation constant of (ZB) VTe bulk

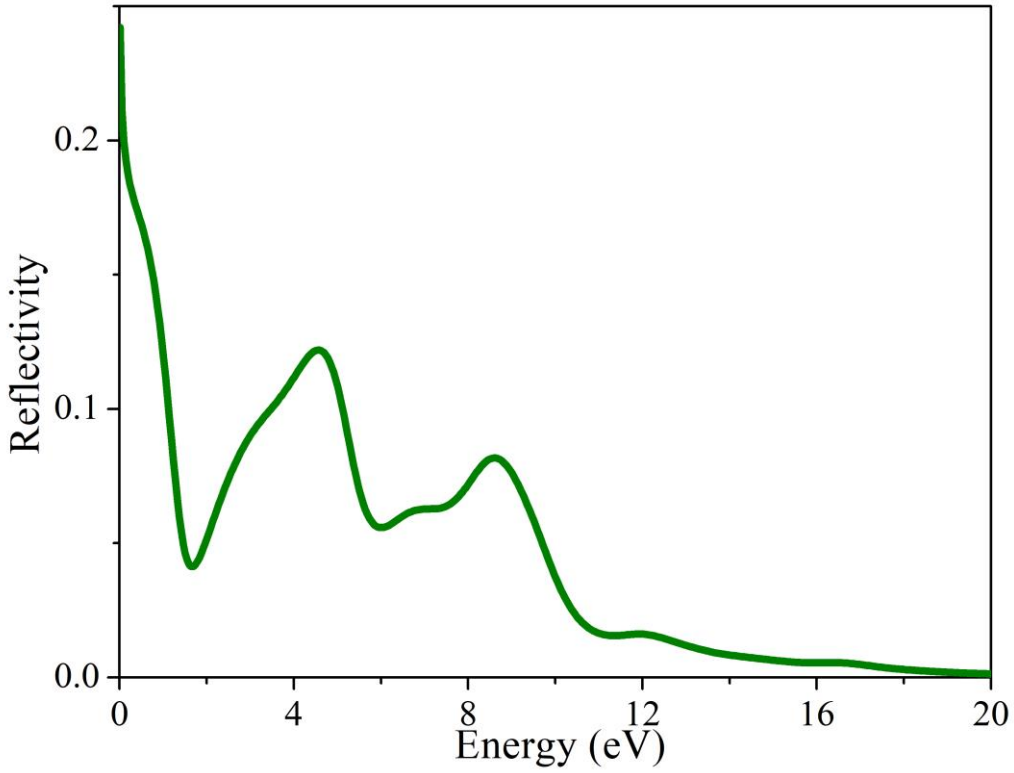


Figure 7: Reflectivity of (ZB) VTe bulk

Figure 7 depicts the expected optical reflectance as a function of energy. At zero energy, optical reflectivity is 0.25.There is a single optically reflective peak for photon energy at 4.5 eV. The optical reflectivity curve decreases with energy in visible light and rapidly decreases with increasing photon energy in ultraviolet light. Based on Figure 8, we can observe that the loss function's maximum peak, with a value of 1.3, occurs at an energy of 10 eV.

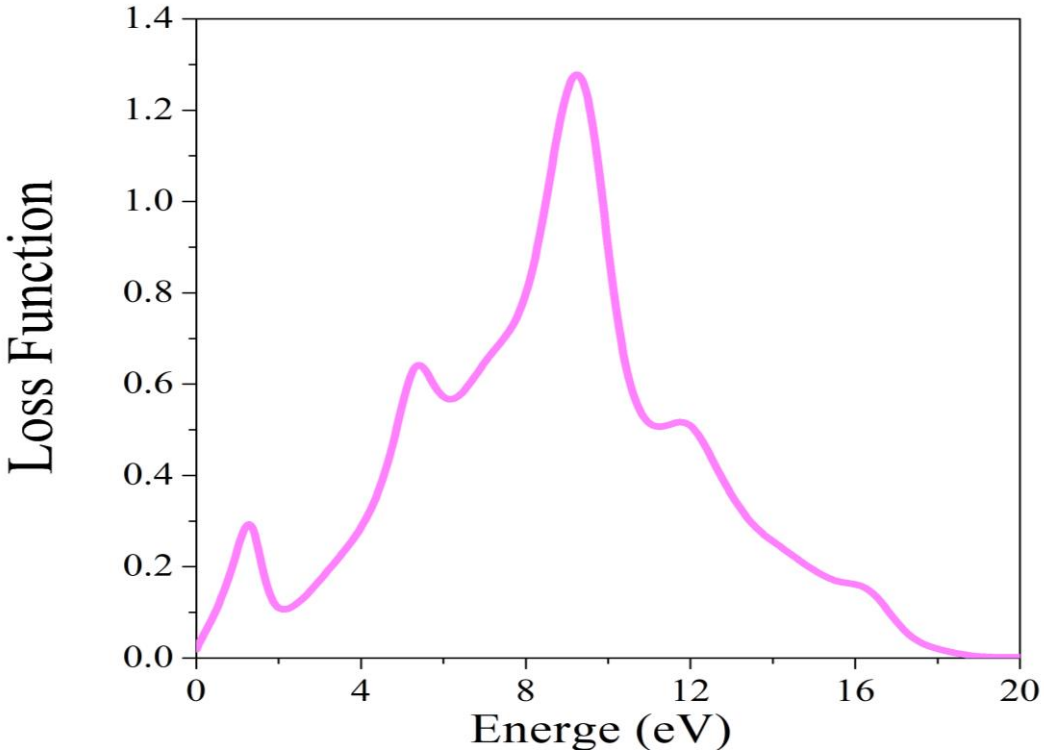


Figure 8: Loss function of (ZB) VTe bulk

Optical conductivity as a function of photon energy is seen in Figure 9. The conductivity of the actual section of the (ZB) VTe bulk peaks at 1.3 eV in the infrared region of 95000. On the other hand, the highest values of the imaginary component of conductivity in the visible ray zone are 65000 at photon energies of 3 eV.

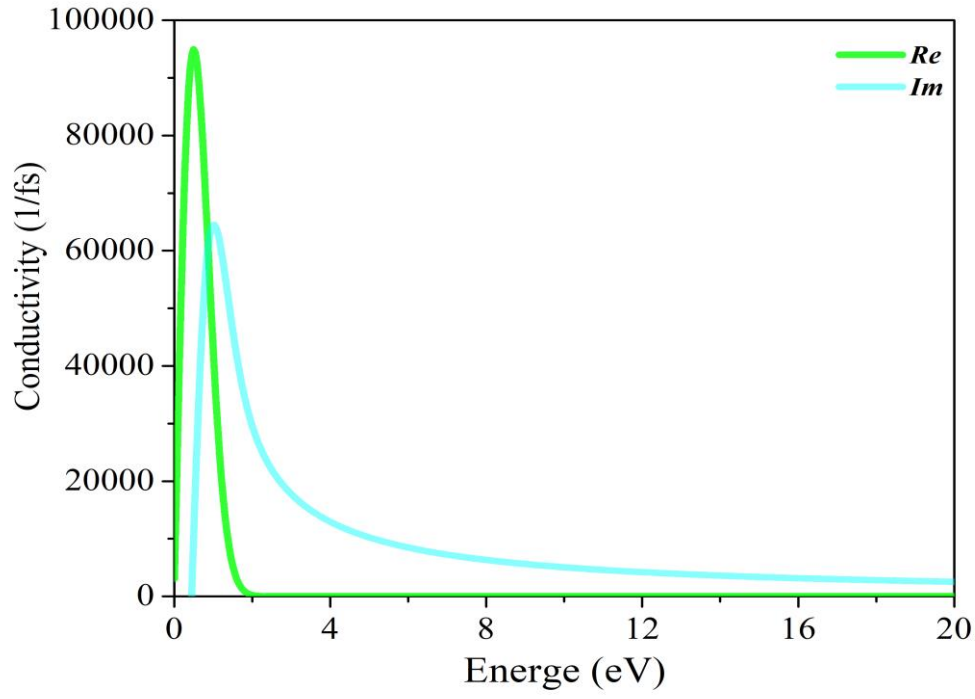


Figure 9: Optical conductivity of (ZB) VTe bulk

CONCLUSION

The (ZB) VTe bulk's electronic structure, optical properties, and phonon transport is all examined in this paper using a first-principles approach. at 15 GPa of applied pressure. Half-metallic features in the (ZB) VTe bulk demonstrate that the spin-up channel is metallic and the spin-down channel is a semiconductor. The average magnetic moment per cell unit in the (ZB) VTe bulk is 3μB. Another factor supporting the dynamic stability of the (ZB) VTe bulk is the absence of imaginary phonon vibration frequencies over the whole Brillouin region. The optical characteristics studied indicate that the (ZB) VTe bulk is a promising candidate for use in microelectronic and electro-optical applications.

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