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Investigate the electrical structure, optical character-characteristics, and phonon transport of the rock-salt (RS) CrTe monolayer using first-principles methods

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ABSTRACT

Density functional theory (DFT)-based first-principles computations are utilized to examine the phonon Boltzmann transport as well as the structural, electrical, and optical characteristics of the (RS) CrTe monolayer. The results demonstrated that the half-metal property is present in the (RS) CrTe monolayer. Whereas in the case of spin-up, the property of metal was achieved because the energy bands cut the level of Fermi, in the case of spin-down, because an energy gap emerged on both sides of the Fermi EF level, the semiconductor was produced. That is, there is a gap between the conduction band and the valence band, and the absolute magnitude of the sum of both gaps indicates to the (RS) CrTe monolayer total energy gap which has a value of 0.902 eV. The magnetic moment per cell unit of an (RS) CrTe monolayer is equivalent to 4μB. The (RS) CrTe monolayer has a strong polarization with a spin equal to 100% at the Fermi level due to the half-mineral. Our findings demonstrate the wide absorption spectrum of the (RS) CrTe monolayer, spanning visible light to the ultraviolet region, as well as its decreased convergent phonon scattering rate. These results could lead to more theoretical and experimental research on the CrTe monolayer's electrical structure, optical properties, and ability to conduct heat.

1. Introduction

In recent decades, spintronic device development has focused on half-metallic (HM) materials due to their indirect applications in electronic device technology. Heusler alloys half-metallic composition intrigues spin-electronic device researchers. These chemicals were first discovered in 1983 by De Groot and his group in type C1b in two semi-hewsler compounds (NiMnSb and PtMnSb) where they were the first alloys to be called half-metal (HM) after which they discovered other alloys applied to that designation (half metal) including full Heusler alloys, $La_{0.7}Sr_{0.3}MnO_3$ alloys and other alloys [1-2]. The unusual properties of some Heusler compounds prompted researchers to study their electronic structure, and some of these alloys showed the properties of metals

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as well as semiconductors or insulators, giving the alloy the name "half of the metal ferromagnetism" according to spin direction. The half-metallic (HM) shows 100% spin polarization at Fermi because the electronic structure is a metal in only one of the two spin channels and is a promising spin-link material. In the past 35 years, first-principles calculations have predicted or confirmed the existence of different semi-metallic ferromagnetic materials [3-7]. Konstantin Novoselov and his team exfoliated graphene from Craft using a mechanical exfoliation method in 2004 [8]. Because of their unique physical, magnetic, optical, mechanical, and electronic properties, ultra-thin 2D nanomaterials have received unprecedented attention. These extraordinary properties have the potential to provide ample space and significant improvements in materials science and innovation [9]. As a result of these sudden properties, graphene and its derivatives are expected to take on enormous potential in optical-electronic devices and many other applications in transistors, nanoscale devices, catalysts,
nano electromechanics, photocatalysis, gas sensors, and optical detectors [10–15]. In recent years, a lot of work has gone into finding reliable ways to make 2D nanomaterials that can be used for different things. Extensively, 2D nanomaterials have been developed using the top-down and bottom-up methods, respectively. In the first method, the van der Waals reaction between the stacked layers of bulk-layered crystals is removed to obtain single-layer or low-layer two-dimensional nanomaterials [16]. Tremendous advances in nanotechnology and materials science have been the reason for the miniaturization of electronic devices, including mobile phones, tablets, computers, and others, and have greatly improved the functionality, stability, and efficiency of these devices. There is no doubt that people's lifestyles have changed due to this technological advancement, as this trend in technology was supported by the Moore Act, which was invented by Gordon Moore, one of the founders of Intel, in 1965. He noted that the number of transistors on the processor chip almost doubles every two years while the chip price remains the same. This observation led to the initiation of the integration of silicon (Si) with integrated circuits by Intel, which contributed to the revitalization of the technological revolution around the world [17]. Silicon, which has been used as a microprocessor for more than four decades, has reached its nanoscale using the quantum tunnel effect principle [18]. There have been many investigations on the surface and interface properties of HM materials, but the majority of these studies do not preserve the surface and interface properties of HM materials [19-22].

2. Computational methods

In this work, the CASTEP code is used in conjunction with density functional theory [23] to calculate the optical properties, magnetic properties, electrical properties, phonon transport properties, and structural properties of the (RS) CrTe monolayer. The PBE technique and the generalized gradient approximations (GGA) have been utilized in order to analyze the exchange-correlation energy [24]. The created system is an (RS) CrTe monolayer that has 15 inserted in a direction that is perpendicular to the surface of the 2D monolayer in order to eliminate any interactions that may exist between atoms. There are (2,2,1) per unit cell in the system. When considering plane waves, the cutoff energy of 500 eV is applied. Every structure has reached its maximum level of relaxation. The atomic force has a magnitude of less than 0.01 electron volts, whereas the total energy affinity has a magnitude of 10^{-6} electron volts. In order to duplicate the structural, electrical, magnetic, phonon transport, and optical features of the (RS) CrTe monolayer, a sample is taken from the first Brillouin zone using a k-point.

3. Results and discussion

3.1. Electronic structures of (RS) CrTe monolayer

Figure (1 a, b) shows the total density of states and electronic band structure for structure rock-salt (RS) (Fm-3m, No. 225). According to the score show that (RS) CrTe monolayer is half a metal (HM) with polarization of a spin equal to (SP = 100%). Where the spin down channel is a semiconductor with an energy gap equal to (0.902 eV), and the spin up channel is metal. While the half-metal gap (HMGap) is (0.416 eV), which is calculated from the Fermi level to the top of the equivalence package. Where the (Te) element is possesses six electrons, two in the S orbital and four in the P orbital that have passed the E_F, making it more effective than the (Cr) element [25].

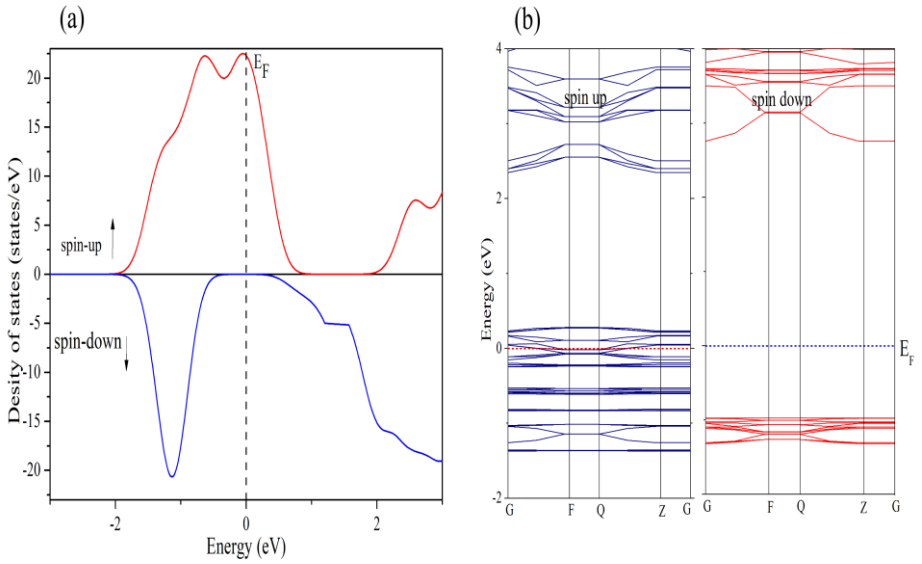

Fig. 1. (a) The densities of states of monolayer CrTe. (b) Band structure (spin↑ and spin↓) of monolayer CrTe.

3.2. Phonon transport

Recent developments in research on materials that are half- metallic materials have emphasized the need for a deeper scientific knowledge of how heat moves through materials. For the purpose of determining the dispersion of the phonon in the (RS) CrTe monolayer, one useful tool is the simulation of calculations of elementary principles based on the theory of functional density (DFT). The study of phonons is an essential component of the physics of materials. This is due to the fact that phonons play an essential role in the formation of many different physical properties, including electrical conductivity and thermal conductivity. In other words, the phonon is the smallest amount of energy that can be transferred from an acoustic source to a physical medium. In this situation, the phonon is like the isotope of electromagnetic waves, which is the smallest amount of electromagnetic energy that can be transferred from an electromagnetic wave to a physical medium [26]. Figure (2) depicts the phonon dispersions of the (RS) CrTe monolayer. This figure demonstrates that the monolayer is dynamically stable because the phonon dispersions lack an imaginary vibrational frequency throughout the entire Brillouin region.

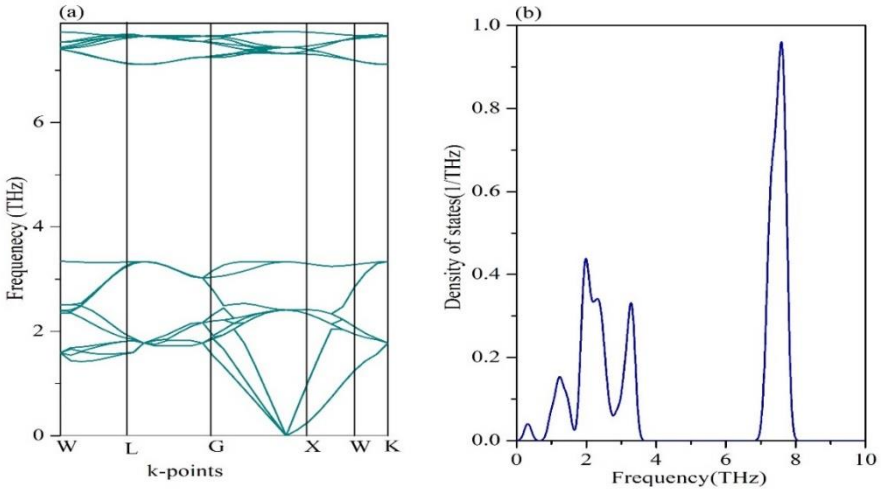

Fig. 2. Curves of phonon dispersion and state density of (RS) CrTe monolayer.

3.3. Optical Properties

Optical properties were studied in the range (0-15 eV) of energy. Where the optical properties of materials play an important role in basic research and modern applications, as two-dimensional materials have helped to improve photovoltaic cells because two-dimensional materials have a larger surface to absorb sunlight, which facilitates the process of light conversion. We calculated the following optical properties: absorption coefficient, reflectivity, loss function, refractive index, propagation constant, conductivity, and dielectric function. Dielectric function is calculated through the following relationship:

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

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 $\varepsilon_1(\omega)$ [27]. The Fermi golden rule is used for adding the occupied–unoccupied transitions to obtain the relationship for the imaginary part $\varepsilon_2(\omega)$ [28].

Figure (3) shows the real and imaginary components of the dielectric function for the (RS) CrTe monolayer. Obviously, the junction of the real component and the vertical axis (at zero energy) is (2500000) and the junction of the imaginary component and the vertical axis (at zero energy) is (6400000). We also note that the true dielectric function is not negative and this indicates that the (RS) CrTe monolayer exhibits semiconductor behaviour in this frequency region. While the insulation curve decreases with the energy in visible areas and ultraviolet radiation with the increase in photon energy. It is well known that materials with gaps below 1.55 eV work well in infrared (IR) radiation and the visible area of the spectrum. So, the (RS) CrTe monolayer will act in the infrared and visible regions as a visual material. [29].

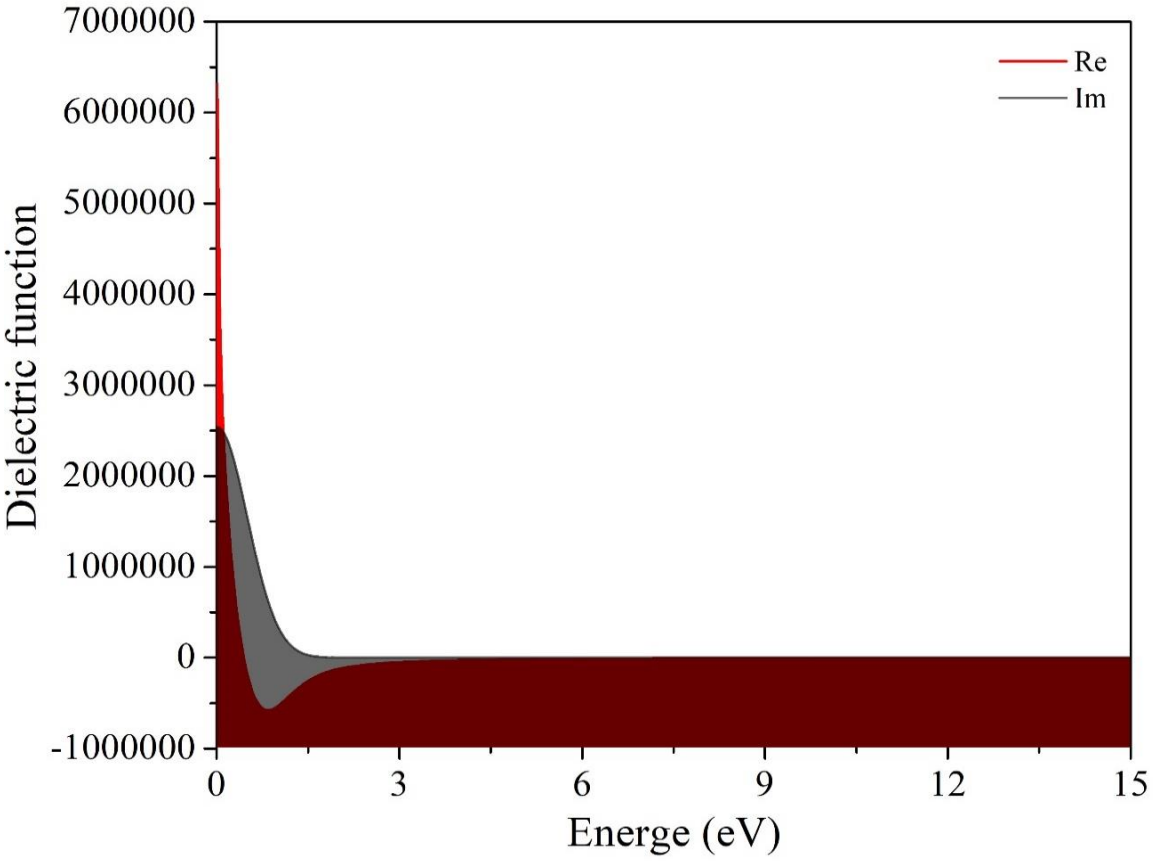

Fig. 3. Imaginary and real components of the dielectric function of the (RS) CrTe monolayer.

Figure (4) shows the Absorption coefficient for the (RS) CrTe monolayer. Where the absorption in the infrared (IR) region begins at less than 0.06eV of the (RS) CrTe monolayer. Regarding the absorption coefficient our results confirmed that there is one absorption peak in the infrared (IR) region in the area between (0.7-1.1 eV). The absorption coefficient shows that its highest peaks are clearly located in the area of ultraviolet radiation 8.25 eV. The absorption of visible light areas begins in the area between (1.6-3.2 eV) and is one of the most important areas for examining the absorption of light that can be used in the manufacture of solar cells. We also note that the (RS) CrTe monolayer possesses a high absorption energy of ultraviolet radiation that can be used in photoelectronic of devices such as UV detectors.

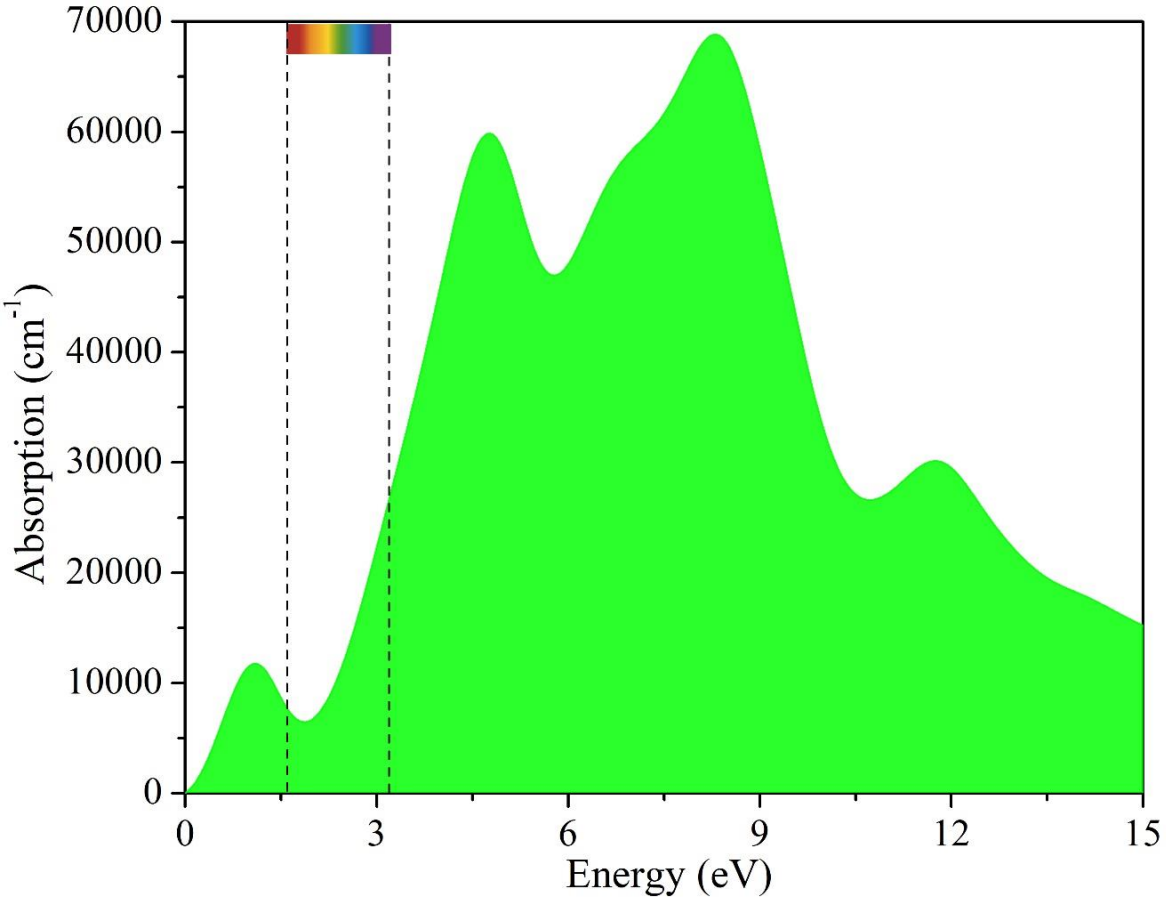

Fig. 4. Absorption coefficient for the (RS) CrTe monolayer.

Figure (5) shows the refractive index and propagation constant of the (RS) CrTe monolayer as a function of photon energy. Obviously, the refractive index and propagation constant (at zero energy) of the (RS) CrTe monolayer are (1500 and 850) respectively. On the other hand, the maximum value of the propagation constant equal 0.76 at 5.62 eV. At high photon energy the refractive index eventually tends to stabilize, while it decreases with energy in visible areas and ultraviolet radiation and in general the mono layer has a maximum refractive index in the Infrared region. The spectrum of refractive index (n) and propagation constant (K) decreases rapidly as the photon energy increases and becomes constant after 15 eV energy.

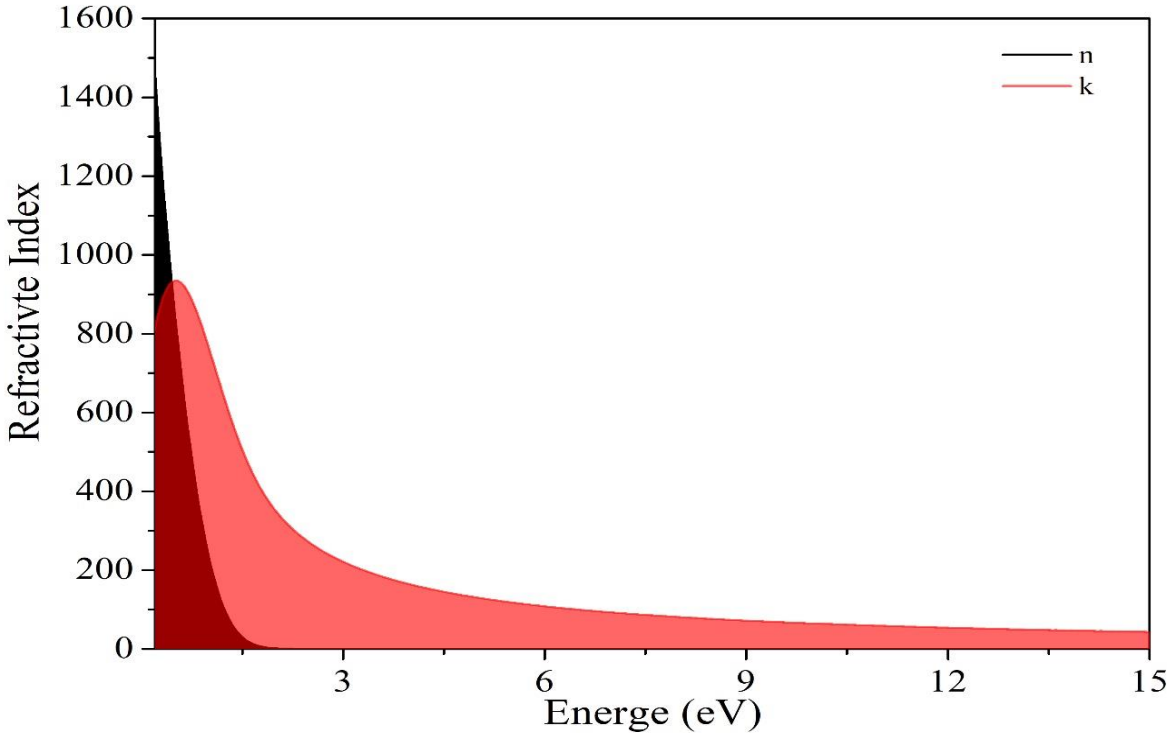

Fig. 5. Refractive index and propagation constant of the (RS) CrTe monolayer.

Figure (6) shows the calculated optical reflectivity as a function of energy. Where we can see through it one optical reflective peak occurs to photon energy at 0.026 eV. The optical reflectivity curve decreases with energy in visible areas and ultraviolet rays as it decreases rapidly as the photon energy increases. Reversive revealed a clear amount of variation in the power range between 0–15 eV and diminishes step by step and becomes almost constant after 15 eV energy.

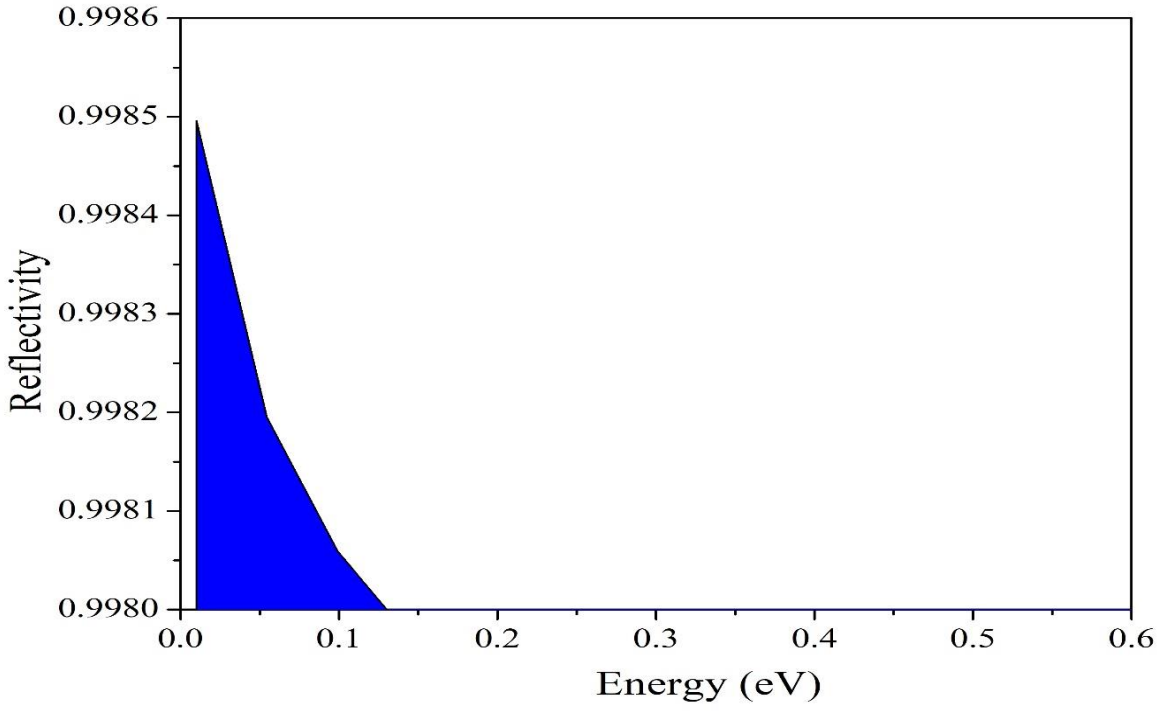

Fig. 6. optical reflectivity as a function of energy of the (RS) CrTe monolayer.

Figure (7) Shows the loss function calculated as an energy function ,where we note that the main sharp peak of energy loss of the (RS) CrTe monolayer is at the photon energy at 13 eV. This energy refers to the transition point between the metal properties to the insulating property of this (RS) CrTe monolayer that can be a good absorber of the medium-low spectrum of radiation. As a result, the current monolayers can be used in solar cell applications.

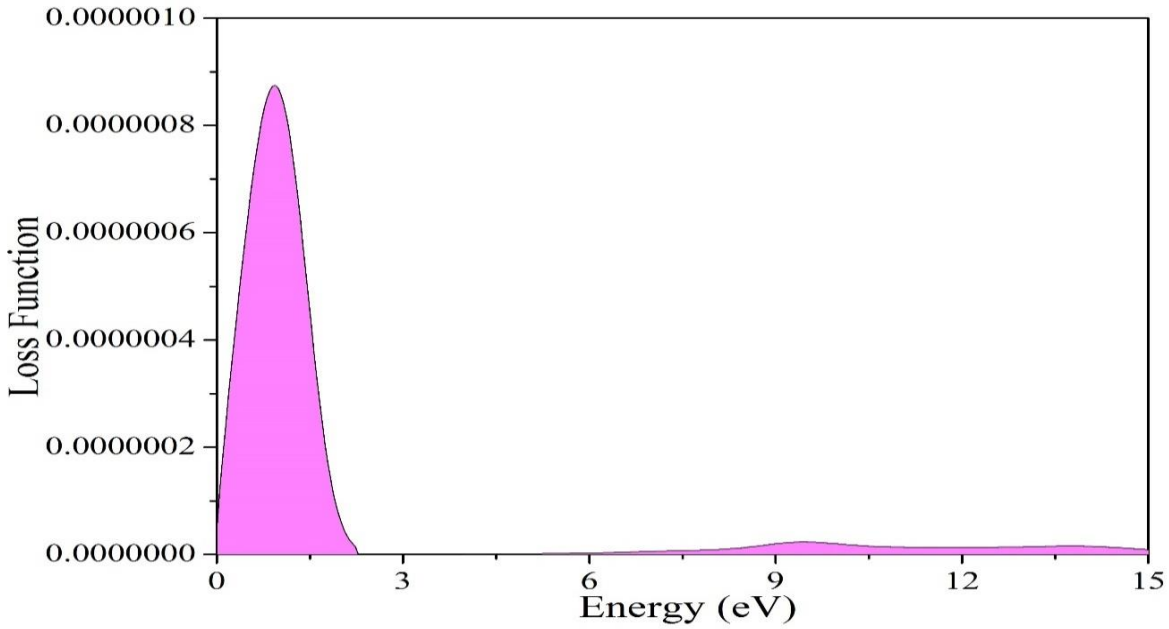

Fig. 7. loss function of the (RS) CrTe monolayer.

Figure (8) shows optical conductivity as a function of photon energy. Obviously, the conductivity of the real part of the (RS) CrTe monolayer has a peak located in the infrared zone of (95000) specifically at 0.76 eV. On the other hand, the maximum values of the imaginary part of conductivity present in the visible ray region are (66000) at the energy of the photon 1.29 eV.

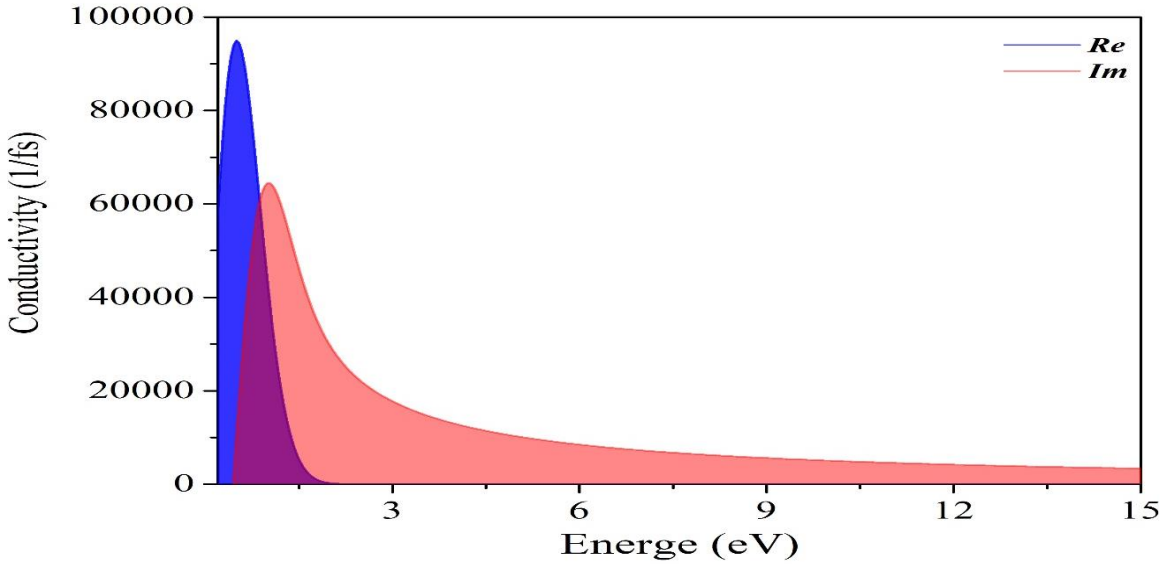

Fig. 8. optical conductivity as a function of photon energy of the (RS) CrTe monolayer.

4. Conclusion

This work considers the electronic structure, optical properties, and phonon transport the (RS) CrTe monolayer through a first-principles investigation. The (RS) CrTe monolayer shows half-metallic properties indicating that the spin up channel is metallic and the spin down channel is the semiconductor with an energy gap equal to 0.902 eV. That the amount of magnetic moment per cell unit of (RS) CrTe monolayer is equal to 4μB. The (RS) CrTe monolayer is also dynamically stable due to the absence of imaginary phonon vibration frequencies in the entire Brillouin region. The studied optical characteristics determine that (RS) CrTe monolayer is a strong competitor for use in microelectronic and electro-optical applications.

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دراسة البنية الكهربائية والخصائص البصرية ونقل الفونون للطبقة الأحادية CrTe للملح الصخري (RS) باستخدام طرق المبادئ الأولى

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الكلمات المفتاحية

نظرية الكثافة الوظيفية ، CrTe ، أحادية الطبقة ، العزم المغناطيسي، الملح الصخري.

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الملخص

تستخدم حسابات المبادئ الأولى القائمة على نظرية الكثافة الوظيفية (DFT) لفحص نقل فونون بولتزمان بالإضافة إلى الخصائص الهيكلية والكهربائية والبصرية لطبقة CrTe أحادية الطبقة (RS). أظهرت النتائج أن خاصية نصف المعدن موجودة في طبقة CrTe أحادية الطبقة (RS). حيث في حالة البرم للأعلى، تم تحقيق خاصية المعدن لأن فجوة الطاقة قطعت مستوى فيرمي، بينما في حالة البرم للأسفل، بسبب ظهور فجوة طاقة على جانبي مستوى فيرمي، تم إنتاج أشباه الموصلات. أي أن هناك فجوة بين نطاق التوصيل ونطاق التكافؤ، ويشير الحجم المطلق لمجموع كلتا الفجوتين إلى فجوة الطاقة الكلية أحادية الطبقة CrTe (RS) التي تبلغ قيمتها 0.902 eV. العزم المغناطيسي لكل وحدة خلية من طبقة أحادية CrTe (RS) يعادلμB4. تتميز الطبقة الأحادية CrTe (RS) باستقطاب قوي مع دوران يساوي 100٪ على مستوى Fermi بسبب نصف المعدن. توضح النتائج التي توصلنا إليها طيف الامتصاص الواسع للطبقة الأحادية CrTe (RS)، التي تمتد من الضوء المرئي إلى منطقة الأشعة فوق البنفسجية، بالإضافة إلى انخفاض معدل تشتت الفونون المتقارب. يمكن أن تؤدي هذه النتائج إلى مزيد من الأبحاث النظرية والتجريبية حول البنية الكهربائية لطبقة CrTe أحادية الطبقة، والخصائص البصرية، والقدرة على توصيل الحرارة.

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