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An Overview of the Electronic Structure of Monolayer Graphene

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ABSTRACT

Monolayer graphene is a nanostructured material that consists of layers of graphene, each layer of single-layer graphene consists of a layer of carbon atoms that are interconnected in a hexagonal lattice. The crystal structure of monolayer graphene is two dimensional and carbon atoms are inserted in a hexagonal lattice. The band structure of monolayer graphene includes two main bands that located at points K and K' considered as quantum bands of electrons and holes. The electronic properties of monolayer graphene include the movement of electrons at very high speed and maintaining their spin. Also, monolayer graphene has unique optical properties and can be used as an optical switcher in electronic devices. Which from the basis of the contemporary technology of graphene and is progressing, therefor, research in this field is important and this research was carried out in a library method and its purpose is to investigate the electronic structure of single – layer graphene.

Keywords- Band, Graphene, Lattice, Monolayer.

I. INTRODUCTION

Statement of the problem: the structure and properties of graphene are among its important and basic features, which include the crystal structure and electronic bands of graphene, its electronic and optical properties. With the passage of time and the advancement of technology, human needs to acquire information and the speed of their processing and storage have increased. In order to better understand nanotechnology, such as the production of transistors of today's generation, we need knowledge to be able to have industrial production of chips in Nano dimensions. Therefore, graphene sheets are composed of carbon atoms, which is the basis of this technology. It is better to check the electronic structure for understanding and clarity. These cases are very important for a better understanding of graphene and its applications in electronic and Nano electronic devices.

The electronic structure of single layer graphene forms the basis of Nano technology and industry, today, the majority of researchers have conducted research in this field and they are trying to produce it, and in the not so distant future, they will include the industry as well. Therefor, the investigation of this structure is very important and necessary. We can find answer by this research to what is the concept of electronic structure of graphene?

Also, about background this research, many researches have been done on the electronic structure of single layer graphene. These researches include theoretical studies, computational simulations and experimental tests. In the following, we refer to some of these studies:

In 2004, the Nobel prize in chemistry was awarded for the discovery of graphene. British researchers obtained these materials by cutting graphite to a thickness of one layer. After analyzing and studying the structure of graphene, they reached interesting conclusions about its electronic properties. They found that single – layer graphene has extraordinary electronic properties (Novoselov et al., 2004). For example, the electrons in single – layer graphene are specifically bound to certain points in the structure, giving the materials unique optical and electrical properties.

In 2010, two researchers from the university of Manchester were able to accurately examine the electronic structure of single – layer graphene using a

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scanning electron micro scoping. They found that electrons in single – layer graphene bind specifically at certain points in the structure. These points are called Dirac points and determine the electronic properties of graphene (Sarma et al., 2011).

In 2015, a researcher from Harvard University was able to accurately examine the electronic structure of single – layer graphene using computer simulations(Liu et al., 2015). He found that the electronic properties of single- layer graphene strongly depend on the shape and size of the nanoparticles in it. These results led to more research on the use of graphene in electronics and nanotechnology. Therefore, this research is also a continuation of the series of researches that have been done and they have focused more on the aspect of the electronic structure of single - layer graphene.

This research was conducted using the library method and its information was collected.

Research goal: investigating the electronic structure of single – layer graphene. In this research, graphene, phonon, polar and transition phonons in graphene, electronic structure of graphene and Auger process in graphene have been investigated and finally a conclusion has been drawn.

II. AN OVERVIEW OF GRAPHENE

Almost 80 years ago, two famous physicists named Landau and Peyrels showed that the two – dimensional lattice is thermodynamically unstable and cannot exist (Landau, 1937). Their theory pointed out that the contribution of thermal fluctuations in the crystal with lower dimensions is of the same order and comparable to the atomic in the lattice points. This argument was then developed by Merman and confirmed by the experimental observations of others (Mermin, 1968).

The study of graphene dates back to the 1960s (Chao et al., 2014). Research in the late 20th century to observe the excellent electrical properties of graphite thin films has been an important work in both theoretical and experimental aspects. It is generally believed that based on theoretical calculations and experimental observations, two – dimensional materials do not exist without a three – dimensional base (Choi & Lee, 2011).

Various attempts have been made to produce graphene, including using the same method to grow carbon nanotubes, chemical vapor deposition on metal surfaces (multilayer graphene), or thermal decomposition of silicon carbide. Although these approaches did not produce flawless monolayer graphene, but research have shown that high mobility exists in multilayer graphene, and the chemical vapor deposition approach has been optimized and has become a major method for today's graphene production (Novoselov et al., 2005).

In fact, the melting temperature of a thin film decreases drastically with the reduction of its thickness, and therefore the thin film becomes unstable in about 12 layers. Until, in 2004, two – dimensional graphene was made by a group of physicists from the university of Manchester, England, led by Andrei Geim and Konstantin Noveslov, using a completely different and natural method and they brought about a change in the investigations related to carbon (Alwarappan & Kumar, 2013). They started with three – dimensional graphite and extracted a single – layer sheet (a single atomic layer) with a method called micromechanical slitting. Because of this the physics' Nobel prize in 2010 was awarded to these two scientists, it has brought great motivation to this issue. Many interesting applications of graphene require the growth of monolayer graphene on bed, which is very difficult to control, after the fabrication of graphene, the research on the control of graphene layers on substrates, the performance of graphene and the applications of graphene have grown exponentially.

Phonon:

Phonons in graphene are phenomena such as sound and light waves that are created there due to the existence of the crystal lattice of graphene (Adamyan & Zavalniuk, 2010). Phonons are actually thermal instabilities in the graphene lattice that cause vibrations in the lattice (Wang et al., 2010). For example, when graphene reaches high temperatures, phonons cause changes in its electronic properties. For example, increasing the temperature decreases the electrical resistance of graphene, which is due to changes in the shape and spatial structure of phonons.

Plural phonons and electron transfer in graphene:

The vibrational properties of graphene show that the phonon scattering is formed by the electron – phonon pair reaction, which leads to the occurrence of two Cohen anomalies in the highest branch of the optical phonon, so the properties of phonons in graphene have attracted the attention of researchers.

Graphene is not a nonpolar material, therefor, currently available graphene samples from polar substrates such as hexagonal boron nitride (h – BN), silicon carbide (SiC), Silicon dioxide (SiO_2), Hafnium dioxide (HfO_2), Aluminum oxide (Al_2O_3) and Subconium dioxide (ZrO_2), they are used for fundamental and applied technology studies. Such polar substrates near the graphene substrate interface, which act as an important scattering source for charge carriers, enable the existence of polarized optical phonons in graphene. Thus, studying the effects of optical surface electron – phonon coupling using the polar substrates that we mentioned before is important for a complete understanding of the change of electronic properties in graphene. Therefore, the optical surface electron – phonon coupling affects the transport properties, which allows scientists to develop quantitative theories for

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many different experimental studies on graphene (Geim & Novoselov, 2007; Rozhkov & Nori, 2010).

Electronic structure of graphene:

The electronic structure of graphene follows the simple nearest neighbor approximation in the tight – binding method. Graphene has two atoms in its simple cell, which results in two conical points for each Brillouin zone, where the energy band crossing occurs at K and K'. near these points, the electron energy is linearly dependent on the wave vector. In fact, this behavior comes from the symmetries of the problem, and therefor the behavior is more dominant than the processes of long range jumps .(Geim, 2011).

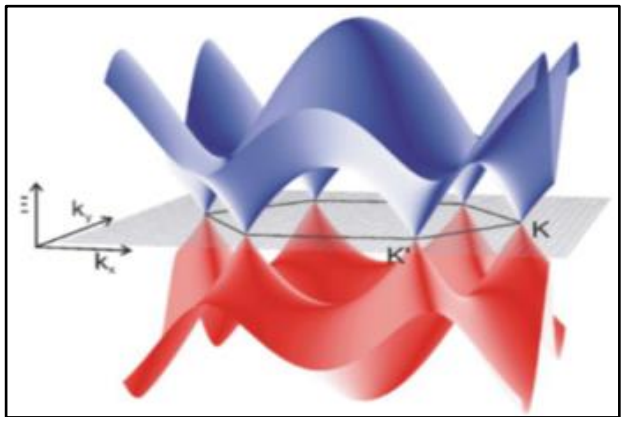
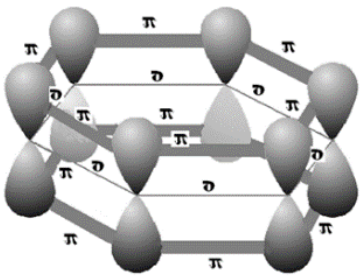


Figure (1): the band structure of graphene, the conduction band intersects with the valence band at points K and K'.

Graphene has a remarkable structure due to its crystalline structure. The configuration of electrons in the carbon atom is such that two electrons are placed in the first orbital and this circuit is completely full, the second orbital also has two electrons, and $2p_x$ and $2p_y$ contain one electron, but in $2p_x$ orbital there isn't any electron. The $1s$ circuit has very little energy, but $2s$ and $2p$ circuits they are very similar in terms of energy. The $2s$, ^2p_x, ^2p_y and ^2p_z together they can have 8 electrons. But they have just 4 electrons in the carbon atom, these four electrons are responsible for chemical bonding, conduction and physical properties. In the one – dimensional graphene layer, there is ^2p_z one more electron in each of the three Hybridized orbitals sp^2 (Yang et al., 2018). Single electrons in the orbital p_z they are perpendicular to the graphene plane, they are relatively free, to move up and down the surface. Carbon atoms form a hexagon in a two – dimensional plane, each carbon atom is about 1.42 A0away from its three neighbors, and each of them shares a σ bond. Bonds σ resulting from overlapping are end - to – end (Yang et al., 2018).

The fourth bond is a π bond oriented in the Z direction (out of surface). This bond is a type of covalent bond in which two rings of one orbital overlap laterally with two rings of other orbitals. This bond is called (π) which is formed from P orbitals. This bond is usually weaker than the σ bond, the end – to – end overlap of the orbitals is easily done and the amount is significant. But the lateral overlap, in order for it to be as good as the end – to – end overlap, requires two atoms to be very close to each other, which the repulsion of the of the nuclei does not allow. This is the reason why the amount of overlap in the lateral mode is less than in the end- to – end mode because of less overlap, π bonds are weaker than σ bonds.it can be said that all the mono bonds are σ and in multiple bonds are a σ bond and other are π, and from the point of view of quantum mechanics, this weakness is the result of less overlap of the two orbitals participating in the bond due to the parallel arrangement of their components. Electrons participating in bonding are called π electrons, this bond doesn't have the ability of rotation; because in the rotation of parallel arrangement of P orbital components, it is destroyed, the π circuit in graphene can be thought of as a pair of symmetric segments around the Z- axis and centered on the nucleus. Each atom has a π bond, which then pairs together to make π and π*, the π filled bond is known as the capacitance band and the π * empty bond is known as the conduction band, according to figure(2a), these bonds are responsible for most of the special electronic properties of graphene. The hexagonal lattice of graphene can be considered as two parts of three triangular lattices figure (2b), what makes graphene so interesting to research is that its spectrum is very similar to the Dirac spectrum for without mass fermions. Dirac's equation describes relativistic quantum particles by ½ spin like electrons. The basic feature of the Dirac spectrum is the possibility of the existence of antiparticles, which is obtained from the principle of quantum mechanics and the theory of relativity. In particular, states with positive and negative energies (electrons and positrons) are positively correlated and described by different components of a spinorily states function (Cooper et al., 2012).



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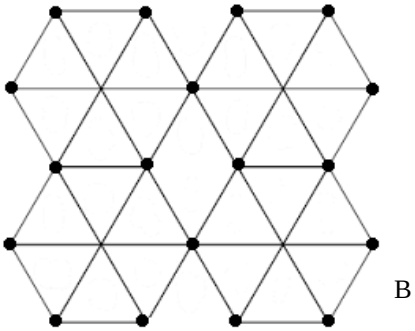

Figure (2): A. types of bonds between carbon particles and fourth bonds. B. graphene's hexagonal lattice, which is considered as two parts of the triangular lattice shape.

This basic features of the Dirac equation is often known as charge – covalent symmetry. For Dirac particles with m mass, there is an energy gap between the minimum energy of the electron $E_0 = mc^2$ and the energy as a positron ($-E_0$). When be electron's energy E E_0, the energy is linearly related to the wave vector $\vec{k}$. For a Dirac fermion without mass the energy's gap is zero and this relationship establishes a linear dispersion $E = v_F \hbar |\vec{k}|$ at each energy (Xu et al., 2018).

In this state, there is an intrinsic connection between spin and particle motion, spin can only be oriented in the direction of propagation (for a particle) or opposite (for an antiparticle). Instead, the spin ½ of the particles can have two image values in any direction. The truth is that we are facing a unique situation here, the electric charge transport in graphene is described similar by Dirac's spectrum and the normal non – relativistic Schrödinger equation can be a result of the crystal structure of graphene. Such as an article compatible with graphene, which is made of two equivalence sub lattices (A) and (B) (Born & Huang, 1996; Semenoff, 1984). Figure (3), the quantum mechanical jump of electrons between two sub lattices causes the formation of two bands and the intersection of these two near the edges of the Brillouin Zone give a conical energy distribution. Similar- particles of graphene show a linear dispersion that if we consider these without of mass particles relativity, the Fermi speed plays the role of the speed of light. Because of the linear spectrum in graphene, similar particles are expected to behave differently than what we know in common metals and semiconductors have that in this state the dispersion relationship is approximated as a sagittal (Semenoff, 1984).

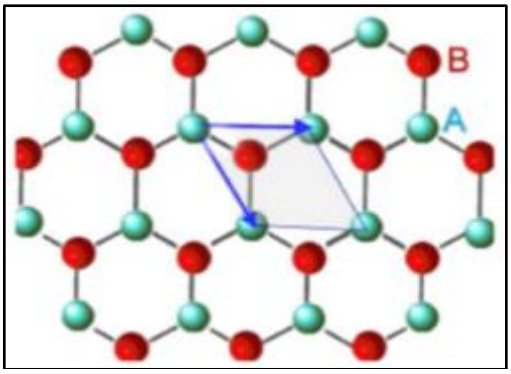

Figure (3): the cognitive crystal structure of graphene, atoms related to different sub lattices(A) and (B) are marked with different colors.

Auger process in graphene:

Researches show that graphene has special optical and electronic properties, which researchers are of great interest in both basic research and industry (Geim & Novoselov, 2007). These properties are related to its linear band structure and unusual energy gap, therefore, opposite of semiconductors that have parabolic bands and band structures, graphene shows an Auger scattering type (Abergel et al., 2010; Neto et al., 2009).

Auger process or Auger scattering is a process which in an atom is ionized through the emission of an electron with energy in the X- ray range, in that the second electron is emitted instead of the X-ray photon. This process has two types, ones is object recombination which is denoted as(AR), second, impact ionized (inverse Auger recombination) is explained in fig(4) (Mahdouani & Bourguiga, 2017).

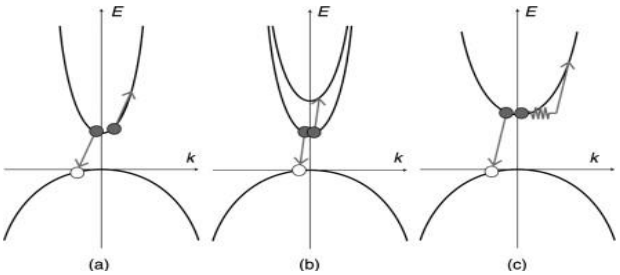

Figure (4): Auger project: A. impact ionization (reverse Auger recombination), with direct Auger recombination.

In which an electron is scattered from the conduction band to the valence band, while at the same time energy is transferred to another electron, which is excited from a higher energy state in the conduction band, is shown in figure(b) above (Mahdouani & Bourguiga, 2017; Winzer et al., 2010).

In the state of impact ionization, an electron is induced into lower energy states, causing an electron to be excited from the valence band to the conduction band, as shown in (a) above. By the same method, both processes also happen for holes. In typical

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semiconductor structures this … channels are created with constraints imposed by conservation of momentum energy. Which is difficult to realize due to band gap and energy dispersion, graphene is expected to exhibit highly efficient dispersion through Auger processes. Direct and inverse sputtering are among the primary processes that lead to the production of hot carriers in semiconductors. These two processes consist of the destruction or generation of electron – hole pairs through energy exchange with accelerated charge carriers or non - accelerated carriers. Auger inverse scattering mode is generally suppressed; because the reduced carriers must have more energy than the band itself. In graphene, which has no energy gap, Auger scattering is predicted to dominate at the first delay time (Brida et al., 2013; Mahdouani & Bourguiga, 2017).

III. RESULT

Polarized and electron transfer phonons in graphene are two types of material movements in this structure, both of which have been studied as important phenomena in the electronic and photonic properties of single – layer graphene. Polar phonons are relatively stable motions in which graphene atoms alternately move toward each other, causing changes in the distance between them. These movements can occur in certain wavelength ranges and with certain frequencies.

Polarized phonons in monolayer graphene, due to its two dimensional structure, have special electronic properties that can be useful in various applications, including electronics and photonics. Single – layer graphene has a special electronic structure and has made this structure known as a very attractive base in electronics and photonics research. In single- layer graphene, electrons are located in two energy bands with Zero energy, which are known as K and K' bands. Both bands have Dirac points, which indicate that electrons in this structure move linearly and at very high speeds.

Also, in single- layer graphene, electrons have special electronic properties due to the existence of a two- dimensional structure, which can be useful in various applications, including electronics and photonics. For example, the electronic properties of single- layer graphene can be used in the production of very fast and low – power transistors, including its electronic applications. Also, due to the special photonic properties of graphene, this structure can be used in the production of LED lamps with high efficiency and in the production of photonic transistors.

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