# Study of Some Electronic Properties of Graphene Sheet by Using Density Functional Theory

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## Abstract

In this work, we investigate the electronic Structure (number of open channels 'NOC', density of states 'DOS' and band structure BS) of graphene sheet using SIESTA and GOLLUM codes. Ab initio structural optimization performs for all structures using the local densityapproximation (LDA) with norm-conserving pseudopotentials, double zeta polarized (DZP) basis sets of pseudoatomic orbitals, and the Ceperley-Alder exchange correlation functional with the atomic forcesrelaxedto0.02eV/A˚.

**Keywords: Graphene ,Density of states, Band structure.**

## 1. Introduction

Carbon demonstrates unusually complicated behavior, forming a number of very different structures. As well as diamond and graphite, which have been known since ancient times, recently discovered fullere- nes and nanotubes [1] are currently a focus of attention for many physicists and chemists. Thus, only 3-dimensional (diamond, graphite), 1-dimensional (nanotubes), and 0-dimensional (fullerenes) allotropes of carbon were known[2]. The two-dimensional form of carbon is named graphene. The discovery of graphene, a single layer of carbon atoms has added a new class of materials to the material family, that of one-atom thick two-dimensional materials. The isolation of two-dimensional graphene from the layered material graphite by using the simple and unusual method of repeated mechanical peeling by scotch tape has stunned the scientific world. The long debate about the existence of two dimensional materials has settled when scientists from the University of Manchester published their first paper about this novel material in 2004[3]. Graphene is a single layer of carbon packed in a hexagonal (honeycomb) lattice, with a carbon-carbon distance of 0.142 nm. It is the first truly two-dimensional crystalline material and it is representative of a whole class of 2D materials including for example single layers of Boron-Nitride (BN)[4]. The electronic structure of graphene is rather different from usual three-dimensional materials[5]. Clean graphene is a semimetal contains a vanishing density of states at the Fermi energy with remarkably high carrier mobility at room temperature and therefore a single-layer graphene can be considered as a semiconductor with zero energy gap or behave as semi metallic material[6].Few layer graphene (FLG) has three to nine layers. The limit where grapheme becomes graphite

is ten layers. The atomic structure of graphene gives rise to exceptional electrical, optical, mechanical and thermal properties [7]. The most interesting electrical properties are high electron mobility and ballistic transport of charge carriers. However, these properties come with a twist; graphene is zero-band gap semiconductor, or semimetal. The lack of band gap in intrinsic graphene is perhaps, together with large scale manufacturing, the most difficult engineering issue[6].

## 2. Theoretical Basis:
## 2.1. Density Functional Theory

One of the key quantum mechanical methods used in physics and chemistry to investigate the electronic structure of many-electron systems it is density functional theory (DFT), in particular molecules based on a strategy of modeling electron correlation via general functional of the electron density . DFT is widely used by physicists and chemists to investigate the ground-state properties of interacting many-particles systems such as atoms, molecules and crystals. DFT transforms the many-body system into one of non-interacting fermions in an effective field. In other words, the electrical properties of many interacting particles system can be described as a functional of the ground-state density of the system [8]. Schrödinger equation Any given non-relativistic many particles system can be described by the time independent, non-relativistic Schrodinger equation[9]:-

$$\hat{H}\,\Psi = E\,\Psi \qquad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (1)$$

$\Psi$ is a wave function called eigenfunction, is the eigenvalue of the Hamiltonian, $\hat{H}$ is the Hamiltonian operator (gives the kinetic and potential energies of a system of atomic. The assumption that the electronic motion and the nuclear motion in

The zero-band gap means that graphene cannot be switched from conductive state to non-conductive state. The lack of a band gap is a problem, if graphene is to be used in logic circuits in much the same way as silicon is used today as the material in complementary metal-oxide semiconductor logic circuits. Nonetheless, the zero band gap of large area graphene is not an issue in all applications[5].

molecules can be separated and called Born-Oppenheimer approximation. The nuclear motion is so much slower than the electronic motion that it could be considered as fixed. The kinetic energy of nuclei is eliminated and the potential energy of nuclei-nuclei could be considered as fixed. In terms of this, the kinetic energy of nuclei and the potential energy of nuclei-nuclei can be eliminated from the Hamiltonian operator, and the Hamiltonian operator $\hat{H}$ is simplified as following [10]:-

$$\hat{H}_{el} = \hat{T}_{e}(r) + \hat{V}_{en}(r) + \hat{V}_{ee}(r) \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots (2)$$

then Schrödinger equation become:

$$\left[\hat{T}_{e}(r) + \hat{V}_{en}(r) + \hat{V}_{ee}(r)\right]\Psi = E\,\Psi \qquad \ldots \ldots \ldots \ldots \ldots (3)$$

DFT provides an appealing alternative, being much more versatile, with $\hat{V}_{ne}$, onto a single-body problem without $\hat{V}_{ne}$. In DFT the key variable is the particle density which for a/Normalisable _wave_function Normalisable wave function $\Psi$ is given by[10]:-

$$\rho_{(r)} = \sum_{i}^{n_i} [\Psi_i(r)]^2 \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (4)$$

Where the summation is over occupied molecular orbitals and ni is the number of electrons in orbital (i).

## 3- Results and discussion

Our calculations are performed by using the SIESTA implementation of DFT[11]. In this work, an ab initio structural optimization was performed for all structures using the local density approximation (LDA) with norm-conserving pseudopotentials, double zeta polarized (DZP) basis sets of pseudoatomic orbitals, and the Ceperley-Alder exchange correlation functional with the atomic forces relaxed to 0.02 eV/A°.Using SIESTA, the density of states 'DOS' was calculated using one k-point in X direction, 200 k-points in Y direction and 200 k-points in Z direction. Next, we calculate the band structures'BS', number of open channels 'NOC' of graphene sheets.
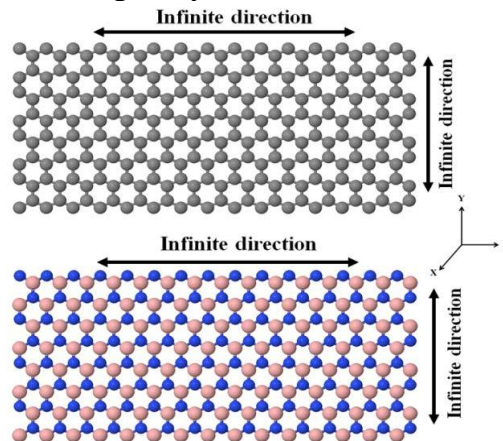


**Figure: (1) shows the relaxed supercell of graphene sheet which contains 240 carbon atoms.**

To understand the electronic properties of the structures in figure 1, we employed SIESTA code to obtain the tight binding hamiltonian (TBH).[12] Later, we calculate the DOS and BS with 1x200x200 k-points. The NOC can be obtained using the non-equilibrium Green's function code GOLLUM, Figure (2) shows the NOC, DOS and BS of graphene sheet.
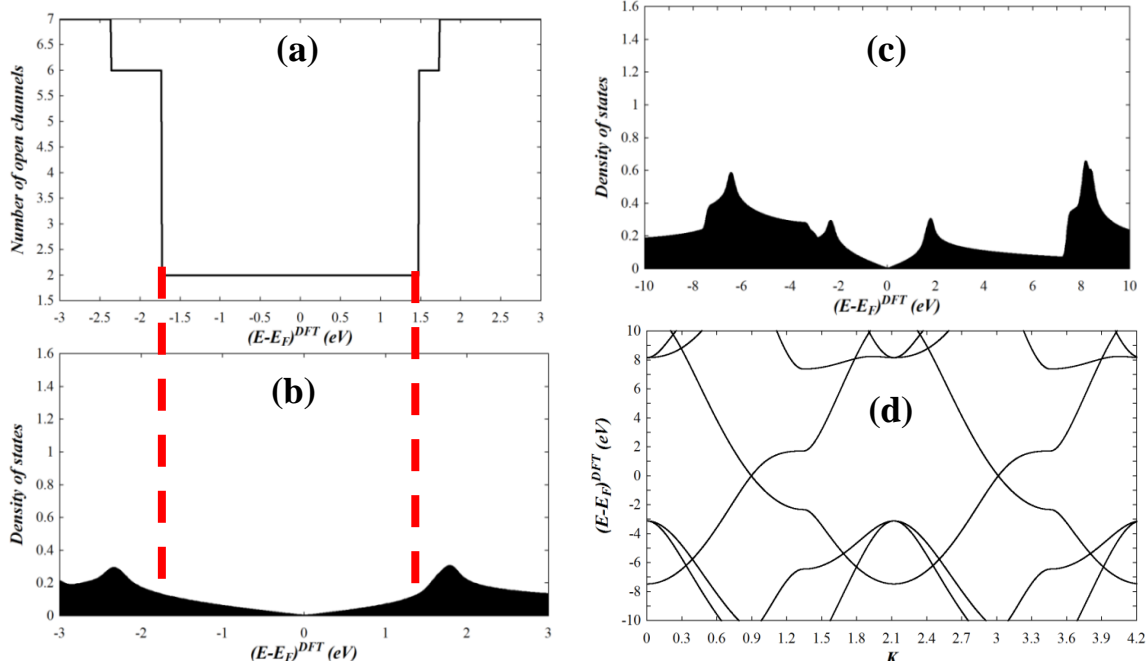


**Figure(2): (a) shows the number of open channels 'NOC' of graphene sheet. (b) and (c) show the density of states 'DOS' of graphene sheet in**

different energy ranges. (d) shows the band structure 'BS' of the structure. All calculations in above carreied out with 1x200x200 kpoints. Looking at figure 2a, we can see that graphene sheet has two open channels at Fermi energy which agrees with publications[13-15].

## 3-Conclusions

Graphene sheet has two open channels at Fermi energy, We can see from figure 2d that there is no energy gap at Fermi energy Due to the zero bandgap of graphene electronic structure, it is not possible to reach high values of the ratio Ion/Ioff between the on state and off state

Figures 2b and 2c show the density of states in different energy ranges and they show that there are available states for travelling electron at Fermi energy. As well as, we can see from figure 2d that there is no energy gap at Fermi energy.

current in graphene field effect devices. To date several strategies have been developed to open a gap in graphene electronic bandstructure, From figures 2b and 2c show the density of states, there are available states for travelling electron at Fermi energy.

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**دراسة بعض الخصائص الالكترونية لطبقة من الكرافين باستخدام نظرية دالة الكثافة**

**الخلاصة:**

في هذا العمل تم دراسة التركيب الالكتروني (عدد القنوات المفتوحة،كثافة الحالة،التركيب الالكتروني لحزم الطاقة) لطبقة من الكرافين باستخدام برنامجي الـ GOLLUM و SIESTA وبالطريقة التامة (ab initio) تم الوصول إلى أفضل تركيب للمركب المدروس بالاعتماد على تقريب الكثافة الموضعية(LDA) والجهد الكاذب والدالة (DZP) تم خفض القوة بين الذرات إلى eV/Aº 0.02.

**الكلمات المفتاحية: كرافين ، كثافة الحالة ، التركيب الالكتروني.**

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