Innovative: International Multi-disciplinary
Journal of Applied Technology
(ISSN 2995-486X) VOLUME 02 ISSUE 03, 2024

The Effect of Doping on The Physical Properties of Graphene

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Abstract:

The presents research focuses on a theoretical study of structural and electronic properties of pure graphene sheet and then adding different number of N_2 atoms . The calculations are carried out using the density functional theory(DFT) was used with hybrid functional B3LYP/6-31G level of theory to investigate the proposed structures. Gauss View 5.0.8 program was used to design the structures of pure and doped graphene sheets. These structures are relaxed by employing the PM6 semi- empirical method with the hybrid functional B3LYP-DFT at Gaussian 09 package of programs. The results of the structural properties of the studied graphene sheets observed that good relaxation of the structures, the values of C-C,C=C, C$\overset{--}{-}$C and C-H bonds in pure graphene sheets remain in the same ranges of the carbon rings structures . These calculations are included the total energy, High Occupied Molecular Orbital HOMO and Low Unoccupied Molecular Orbital LUMO energies, forbidden energy gap, ionization energy and electron affinity, electrochemical hardness, electronic softness. The result of the total energy of the studied doping graphene sheets is a reflection of the binding energy of each structure and indicates to that these structures have good relaxation, and the effect of adding N_2 atoms in pure graphene sheet on the total energy of the molecule is effective. We showed all doping graphene sheets have small forbidden energy gap, but it vibrates depending on the length and number of each sheet and position of N_2 atoms in the sheets. The ionization energy IE and electron affinity EA of the doping graphene sheets are slightly decrease with decreasing the length of the sheets. And all doped graphene sheets have low values of IE and EA in comparison with the pure. Also, we showed that all the pure and doped graphene sheets have low electrochemical hardness H and high electronic softness S. High electronic softness is the main future as a sign for that band gap of the structure goes to be rather soft.

Keywords: density functional theory(DFT), N_2 atoms

Introduction

Graphene is a combination of graphite and the suffix-end, named by Hanns-Peter Boehm, who described single-layer carbon foils in 1962 [1] . It is the basic structural element of other allotropes, including graphite, charcoal, carbon nanotubes and fullerenes[2]. Andre Geim and Konstantin Novoselov at the University of Manchester won the Nobel Prize in Physics in 2010 for groundbreaking experiments regarding the two-dimensional material graphene[3,4]. The carbon atoms in graphene are compactly crowded in a chicken wire regular atomic-scale pattern. Each atom has four bonds of about 1.42 Å, one type of σ-bond with each of its three neighbors and one type of π-bond in which it is oriented out of plane [5]. Graphene can be considered an (infinite) alternant (only six-member carbon ring) polycyclic aromatic hydrocarbon[6]. The term graphene should be used only when the reactions, structural relations or other properties of individual layers are discussed[7,8]. Graphene is reformed with oxygen and nitrogen atoms containing functional groups and analyzed by the infrared spectroscopy and X-ray[9]. However, the strength of character of structures of graphene with oxygen and nitrogen atoms needs high controlling of the structures [10]. Different geometrical terminations of

the graphene monolayer give rise to two different edge geometries of largely varying electronic properties, namely zigzag and armchair graphene[11]. GNRs also called nano-graphene ribbons or nano-graphite ribbons have one-dimensional structures with hexagonal two dimensional carbon lattices .The atoms at the edges of a graphene sheet have unusual chemical reactivity. Graphene has high ratio of edge atoms of any allotrope, defects within a sheet increase the chemical reactivity of the graphene[12-13]. The electronic properties of mentioned materials could be tailored by controlling doping parameters. Doping is a powerful way to modify the properties of graphene-like materials. Spectroscopy and microscopy have been used to characterize doped graphene. Doped graphene could be used in electronics, energy storage, and bio-devices [14]. Doping of semiconductor is necessary for various device applications. Exploiting chemistry at its reactive edges was shown to be an effective way to dope an atomically thin (GNR) for realizing new devices in recent experiments [14, 15]. The high mobility of graphene, which is a monolayer of carbon atoms packed into a two-dimensional (2-D) honeycomb lattice, has stimulated strong interest in high-performance graphene device applications [16]. For n-type doping, substitution of edge carbon atoms by nitrogen atoms is considered, and passivation of edge carbon atoms by oxygen atoms is considered for p-type doping [17]. Nitrogen is the chemical element with the symbol N and atomic number 7 . Nitrogen is the lightest member of group 15 of the periodic table, often called the pnictogens. It is a common element in the universe, estimated at about seventh in total abundance in the Milky Way and the Solar System. A nitrogen atom has seven electrons ,in the ground state, they are arranged in the electron configuration . It therefore has five valence electrons in the 2s and 2p orbitals, three of which (the p- electrons) are unpaired[18]. It has one of the highest electronegativity among the elements (3.04 on the Pauling scale), exceeded only by chlorine (3.16), oxygen (3.44), and fluorine (3.98). Nitrogen gas is also used to provide an unreactive atmosphere. It is used in this way to preserve foods, and in the electronics industry during the production of transistors and diodes. Large quantities of nitrogen are used in annealing stainless steel and other steel mill products. Annealing is a heat treatment that makes steel easier to work [19] [20]. Nitrogen gas has a variety of applications, including: Filling automotive and aircraft tires due to its inertness and lack of moisture or oxidative qualities, as compared to air

As a propellant for draft wine, and as an alternative to or in combination with carbon dioxide in carbonated beverages . Yanwa et al., in 2010[21], interest in graphene excellent physical properties, chemical tenability, and potential for applications has caused thousands of publications and an speed up space of research. This study is an overview of the preparing and studying the properties and applications of the grapheme and related materials, such as graphite oxide and its colloidal suspensions and materials made from them. Masahiro Sakurai, et al In 2011, [22], used the local density approximation within the framework of the density functional theory to study of the electronic properties of graphene with periodic structural modifications. In addition, they observed the lattice composed of graphene and boron-nitride layers show interesting electronic properties being different from those of grapheme in which the material is found to be metallic even though each graphene layer is sandwiched by insulating B/N compound. M. Gautam and B. Harihar , in 2012[23], used the full density functional theory calculations to investigate the structural properties and the electronic properties of graphene and graphene- like materials, viz., monolayer of Si/C, Ge/C, B/N, Al/N. Xiaolin Li et al., in 2012 [24-29] developed a chemical route to produce (GNR) with width below 10 nanometers, as well as single ribbons with varying widths along their lengths or containing lattice-defined graphene junctions for potential molecular electronics. The GNRs were solution phase-derived, stably suspended in solvents with non-covalent polymer functionalization, and exhibited ultra-smooth edges with possibly well-defined zigzag or armchair-edge structures. Aims of The Study was focuses on studying the effect of the length of the ribbon and the addition of the Nitrogen atoms on the structural, electronic properties of (GNRs) using the efficiency density functional theory together with large basis sets 6-31G depending on the hybrid functional B3LYP to determine the paths of the applications of the new constructed structures.

Methodology

The Schrödinger equation, which was named after Erwin Schrödinger who discovered it in 1926, is believed to be the fundamental equation to describe the motions of atomic and subatomic systems, electrons and nucleus, even macroscopic systems as large as the universe. The time dependent form of Schrödinger equation is as the following equation [29]:

$$i\hbar \frac{\partial}{\partial t} T(\vec{r},t) = -\frac{\hbar^2}{2m} \nabla^2 T(\vec{r},t) + V(\vec{r},t)T = H(\vec{r},t)T(\vec{r},t) \qquad (2.1)$$

As

$$\hat{H}T(\vec{r},t) = ET(\vec{r},t) \qquad (2.2)$$

Where Ψ is the wave function, ^H is the Hamiltonian operator, and E is the total energy of the system. The Hamiltonian operator, H consists of two terms the kinetic energy of the electrons and the nuclei (T) and potential energy components (V) as follows:

$$\hat{H} = \hat{T} + \hat{V} \qquad (2.3)$$

The total Hamiltonian of the molecular system H^ containing M nuclei and N electrons can expressed as follows [30, 31]:

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{A=1}^{M}\frac{1}{2m_A}\nabla_A^2 - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} + \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{r_{AB}} \qquad (2.4)$$

$$\hat{H}_{total} = \hat{T}_e + \hat{T}_n + \hat{V}_{ne} + \hat{V}_{ee} + \hat{V}_{nn} \qquad (2.5)$$

In equations (2.4) and (2.5), the total kinetic energy is the sum ofthe electronic ($\hat{T}_e$) and nuclear ($\hat{T}_n$) kinetic energies, the total potential energy are the sum of three components: the attractive interactions between nuclei and electrons ($\hat{V}_{ne}$), the repulsive electron-electron interactions ($\hat{V}_{ee}$) and the repulsive interactions between the nuclei ($\hat{V}_{nn}$). $Z_{A,B}$ are the nucleic charge of atoms A and B, m_A is the mass of atom A, r_{AB} is the distance between nuclei A and B, r_{iA} is the distance between nucleus A and electron i and finally r_{ij} is the distance between electrons i and j, $r_{ij} = |\vec{r}_i - \vec{r}_j|$.

Hartree-Fock Theory

Hartree-Fock theory is the basis of molecular orbital Hartree-Fock theory. It is based on a simple approximation to the true many-body wave function. [31, 32]. Hartree made such a simplification in 1928 through an iterative self-consistent field 'SCF' method. Having this assumption it was possible to proceed using the variational principle. According to the variational principle [31, 33], if a given system is described by a set of unknown parameters the set of parameter values which correctly describes the ground state of the system is just that set of values which minimizes the total energy. This can be expressed as [33, 34]:

$$E_{\emptyset} = \frac{\langle\Phi|\hat{H}\Phi\rangle}{\langle\Phi|\Phi\rangle} \geq E_o \qquad (2.6)$$

Where E_{Φ} is the lowest-energy eigenvalue of the trial function, Φ trial function and E_0 is the ground-state energy. Solving the Hartree-Fockequation using the iterative process of the self-consistent-field (SCF) producer yields the molecular orbitals ψ (r_i) [32, 35, 36]:

$$F\Psi_i(\vec{r}) = \varepsilon_i\Psi_i(\vec{r}) \qquad (2.7)$$

The resulting value of the energy will then be as close as possible tothe exact energy E_o of the ground state of the system within the selected limitations.

$$E(\Phi_1, \Phi_2, \ldots \ldots, \Phi_N) \geq E_o \qquad (2.8)$$

The equality sign shall be applied only in case that, Ψ_i is the exact groundstate function [37]

Basis Set

A basis set is a set of functions used to describe the shape of the orbitals in an atom .When ab initio or density functional theory calculations are done, a basis set must be specified, Molecular orbitals and entire wave functions are created by taking linear combinations of basis functions and angular functions [35, 38].

Slater Type Orbitals (STO's)

The slater type orbitals have the form [39, 40]:

$$\chi^{ST0} = N r^{n-1} e^{-\pounds r} Y_{lm}(\theta, \varphi) \qquad (2.9) .$$

Here n, is a principal quantum number and ξ is a constant related to the effective charge of the nucleus. Y_{lm} is a spherical harmonic whichdescribes the angular part of the wave function.

Gaussian Type Orbitals (GTO's)

Gaussian type orbitals (GTOs) can be written in terms of Cartesiancoordinates as [32, 35, 38]:

$$\chi^{GT0} = N x^{lx} y^{ly} z^{lz} e^{-\pounds r2} \qquad (2.10)$$

N is a normalization factor. The sum of lx, ly and lz determines the typeof orbitals. ξ Represents the orbital exponent that show compact large ξ ordiffuse small ξ is the resulting function. r^2 dependence in the exponentialis a deficiency of the GTO's with respect to the Slater-type orbitals STO's.

Minimal Basis Sets

The minimal basis sets represent all orbitals up to and including valance, it is the minimum number of basis functions χ needed to describe the ground states of the component atoms in a molecule for example (1s, 2s and 2p on carbon atom) [41, 42].

Split-Valence Basis Sets

A split-valence basis sets the inner-shell atomic orbitals are represented by one basis function and the valence orbitals are represented by two or more basis functions (Pople basis sets) [34, 37, 43].

Polarization and Diffuse Functions

Polarization functions are functions of higher angular momentum suchas d- and f- type functions for heavy atoms and p- and d-type functions forhydrogen and helium atoms [38, 44, 45]. Diffuse functions denoted by '+'. For instance, the 6-31++G (d, p) basis set includes a set of d-type functions on all heavy atoms and p-type functions on hydrogen and helium. The first'+' indicates that diffuse s-and p-type functions are included on heavy atoms, while the second '+' indicates that diffuse s-type functions have been included on hydrogen [42, 44].

Density Functional Theory

The density functional theory provides the ground state properties of a system, and the electron density plays a key role. It is presently the most successful (and also the most promising) approach to compute the electronic structure of matter. An example: chemistry. DFT predicts a great variety of molecular properties; molecular structures, vibrational frequencies, atomization energies, ionization energies, electric, magnetic properties and reaction paths, etc. In 1927, the functional predecessor to density theory was the Thomas-Fermi model, developed by Thomas and Fermi [29, 31, 35].

DFT derives properties of a many particle system as a functional of electron density ρ(r). Electron density is the number of electrons per unit volume for a given state. It is dependent only on three coordinates regardless of the number of electrons of the system, so [35]:

$$N = \int \rho(\vec{r})d\vec{r} \qquad (2.11)$$

The fundamental concepts of DFT rely on the ground state energy and all other ground state electronic properties are uniquely determined by the electron density.

The Hybrid Functional

The hybrids functional are very successful in describing a wide range of molecular properties accurately. In large molecules and solids, however, calculating the exact (Hartree-Fock) exchange is computationally expensive, especially for systems with metallic characteristics. In the present work, a new hybrid density functional was draped based on a screened Coulomb potential for the exchange interaction which circumvents this bottleneck.

The most popular hybrid functional, B3LYP, [46, 47], uses Becke's 1988 exchange functional (E_K^{B88}) and Lee, Yang and Parr's

correlation functional (E_C^{LFP}) as gradient corrections to the exchange andcorrelation functional [48].

$$E_{KC}^{B3LFP} = (1-a)E_K^{LSDA} + aE_{KC}^{\lambda=0} + bE_K^{B88} + cE_C^{LFP} + (1-c)E_C^{LSDA} \qquad (2.12)$$

Where the three parameters, a=0.20, b=0.72 and c=0.81.Here

Computed properties

All calculations in this study are carried out by Koopmans theorem .

HOMO, LUMO and Energy Gap

The two most important molecular orbitals MOs are called the frontier orbitals in which they lie at the outmost boundaries of the electrons of the molecules, these MOs are the highest occupied molecular orbital HOMO and the lowest unoccupied molecular orbital LUMO. The band gap is the difference of the energies between the two orbitals HOMO and LUMO[49-51].

$$E_{gap} = E_{LUM0} - E_{H0M0} \qquad (2.13)$$

The energy gap helps not only to control the way the moleculeinteracts with other species, but also to describe the chemical reactivity and the stability of the molecule.

Ionization Energy (IE)

The ionization energy for a molecule is the amount of energy requiredto remove an electron from an isolated atom or molecule [46].

$IE = -E_{HOMO}$ (2.14)\

Electron Affinity (EA)

The electron affinity of a molecule or atom is the energy changewhen an electron added to the neutral atom to form a negative ion [46].

$EA = -E_{LUMO}$ ……… (2.15)

Total Energy (E_{total})

The total energy is the sum of total kinetic and potential energy, at the optimized structure where the total energy of the molecule must be at the lowest value because the molecule is at the equilibrium position, which means, the resultant of the effective forces is zero [46].

Chemical Hardness (H)

In terms of ionization energies and electron affinities, the hardnessis half of the energy gap between two frontier orbitals [52, 53]:

$H= (IE-EA) / 2$ (2.16)

Chemical Softness (S)

The soft molecule has a small energy gap. A small energy gap means small excitation energies to the manifold of excited states. Their electron density changes easier than a hard molecule, and due to that, soft molecules will be more reactive than hard molecules [53].

Results and Discussion

the designing Zigzag Graphene Sheets at Nano Tube Modular program and calculated their structural, electronic properties . All these structures are built by Gaussian View 5.0 and resultsobtained by Gaussian 09 package for structural and electronic proprieties on basis set (6-31G) at hybrid function (B3LYP). Firstly we listed thepure structural with proprieties and adding (N_2) atom(1,2,4,8) to the pure Graphene ribbons . Finally the electronic proprieties studied for (IE, EA,S, H, HOMO, LUMO , E_T and Eg).

Structural Proprieties for Pure Graphene Sheets

Table (3-1) show the bond length and bond types for pure ribbon in Angstrom unit, all these results of bond length are compared with stander model for bond types and their length. The optimization parameters of pure graphene sheet was obtained by DFT calculation of bonds length, weshow also have good agreement with experimental studies for bonds, the range of bonds of (C-C), (C=C), ($\mathrm{C}\overset{\cdots}{-}\mathrm{C}$) and (C-H) are (1.45478– 1.47808) Å, (1.34793– 1.38478) Å, (1.39168– 1.44396) Å and (1.08155–1.08633) Å respectively, this results back to symmetrical distributions of Carbon atoms and Hydrogen in pure ribbon [54]. Figure (3-1) show geometrical structure for ribbon under study.

Table (3-1): Show the bond types and length for stander ribbon.

Graphene Sheet	Bonds	Values Å
Pure	**$\mathrm{C}\overset{\cdots}{-}\mathrm{C}$**	**1.44396**
	C-H	**1.08633**
	C=C	**1.38478**
	C-C	**1.47808**

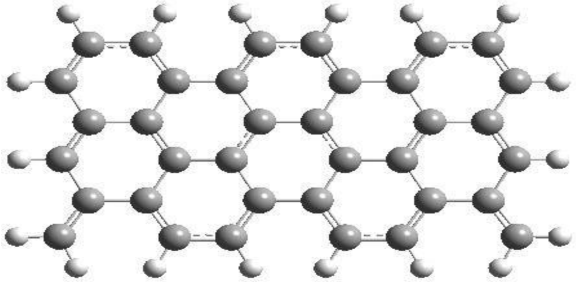
Graphene Sheet	Structure
Pure	

Figure (3-1): Geometrical structure for Pure Graphene Sheet.

Electronic Proprieties

Total Energy, Electronic States and Energy Gap

From table (3-2) contain the Total Energy (E_T), Higher Occupation Molecular Orbital (HOMO), Lowering Inoccupation Molecular Orbital (LUMO) and Energy Gap (E_g) in electron volt unit (eV).

Table (3-2) :Show the Total Energy (E_T), (HOMO), (LUMO) andEnergy Gap (E_g).

Graphene Sheet	HOMO (eV.)	LUMO (eV.)	Eg (eV.)	E_T (eV.)
Pure	-3.73661	-3.46287	0.273743	-37616.3

Ionization Energy (IE) and Electronic Affinity (EA)

The Ionization Energy (IE) and Electronic Affinity (EA) changes values depend on HOMO and LUMO energy, also changes in energy gap. The values of (IE) and (EA) listed in table (3-3) in electron volt unit.

Table (3-3): The values of (IE) and (EA) energy.

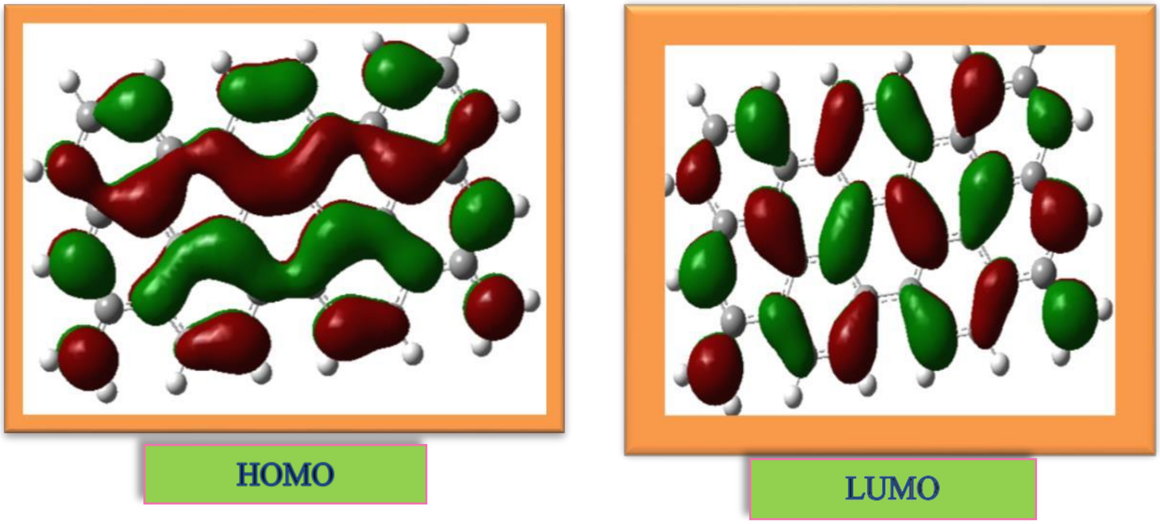
Graphene Sheet	IE (eV.)	EA (eV.)
Pure	**3.73661**	**3.46287**

Chemical Hardness (H) and Chemical Softness (S)

The Chemical hardness (H) and Chemical Softness(S) determine typeof energy gap and ability to reaction with surrounding system . The table (3-4) show result of stander ribbon. Figure (3.2) show the 3-D shapes of HOMO and LUMO distributions of Pure Graphene Sheet.

The table (3-4): Shows result H and S of pure GrapheneSheet

Graphene Sheet	Hardness (eV.)	Softness eV^{-1}
Pure	**0.13687**	**3.6531015**



HOMO

LUMO

Figure (3.2): The 3-D shapes of HOMO and LUMOdistribution of pure Graphene sheet

Adding Nitrogen atoms to Pure Graphene Sheet

In this case we adding Nitrogen atoms to pure Graphene sheet cross the surface of graphene instead of Carbon atoms and study the structural and electronic proprieties.

Structural Proprieties

Table (3-5) show the bond length and bond types for graphene sheets after adding Nitrogen atoms in Angstrom unit, all these result of bond length are compared with stander model for bond types and their length. The optimization parameters of each graphene ribbons were obtained by DFT calculation of bonds length. The bond length for (C-C), (C=C), ($C\overset{\cdots}{-}C$), (C-H) (N_2-N_2) and (C-N_2) are (1.44916-1.48542) Å, (1.36913-1.38583) Å, (1.38648-1.44476) Å, (1.07000-1.08632) Å,(1.36776-1.43782) and (1.42021-1.42158) Å respectively. All values of (C-C), (C=C), ($C\overset{\cdots}{-}C$) and (C-H) are agreement with stander range approximately, for (C-N_2) bond we show obtained single bond this backto fact we have 1 free electrons come from Nitrogen atom sharing in two pair of electron to form single bond between Carbon and Nitrogen and this values agreements with stander values of bond length [55].

Table (3-5) bond length and types in Angstrom unit.

Ribbons	Type	Length Å
	C-N_2	1.43412
	C=C	1.38583
	C-C	1.47263
	C-H	1.08632
	$C\overset{\cdots}{-}C$	1.44476
2	C- N_2	1.43782
	C=C	1.38372
	C-C	1.48542
	C-H	1.08593
	$C\overset{\cdots}{-}C$	1.44211
3	C- N_2	1.42108
	N_2- N_2	1.42158
	C-H	1.07000
	$C\overset{\cdots}{-}C$	1.42158
4	C- N_2	1.42158
	N_2- N_2	1.42158
	C-H	1.07000
	$C\overset{\cdots}{-}C$	1.42158

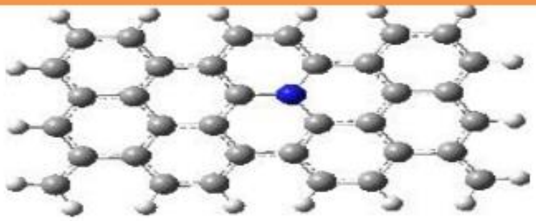
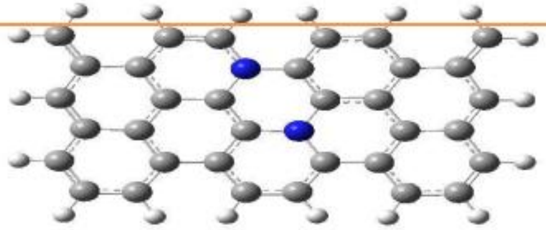
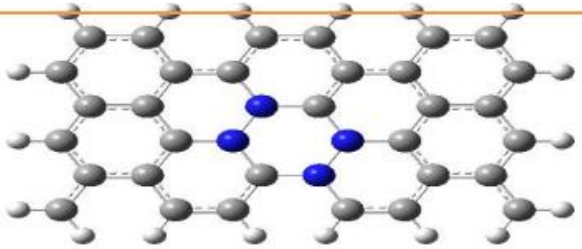
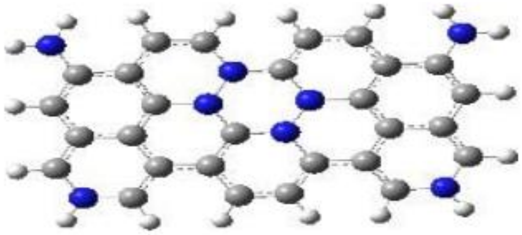
Ribbons	Structures
1	
2	
3	
4	

Figure (3-3): Geometrical structure for ribbons under study.

Table (3.6): show E_{total}, E_{HOMO}, E_{LUMO} and E_g in eV of the Graphenenanoribbons after adding. We show the total energy is decreasing with increasing the number of Nitrogen atoms to the ribbon, the electronic states HOMO and LUMO and have small energy gap compared with pure sheet that refer to ability to translation electrons cross energy band . Figure (3-5 , 3-6, 3-7 and 3-8) respectively show the total energy, electronic states and energy gap for graphene ribbon after adding Nitrogenatoms.

Table (3.6): E_{total}, E_{HOMO}, E_{LUMO} and E_g in eV of the GNRs.

Ribbons	Etotal(eV)			Eg(eV)
		EHOMO(eV)	ELUMO(eV)	
1	-38068.35	-3.26831	-2.29797	0.97034
2	-38519.06	-3.62097	-3.04301	0.57796
3	-39419.75	-6.59159	-2.35593	4.23566
4	-41230.76	-2.55258	-1.443	1.10958

Figure (3.5) show that, the presence of Nitrogen atoms at the terminal ends of phenylene rings in each ribbon leads to decrease the total energy of the ribbon. The difference in energy between the structures 1 and 2 is approximately the same as between the structures 3 and 4.

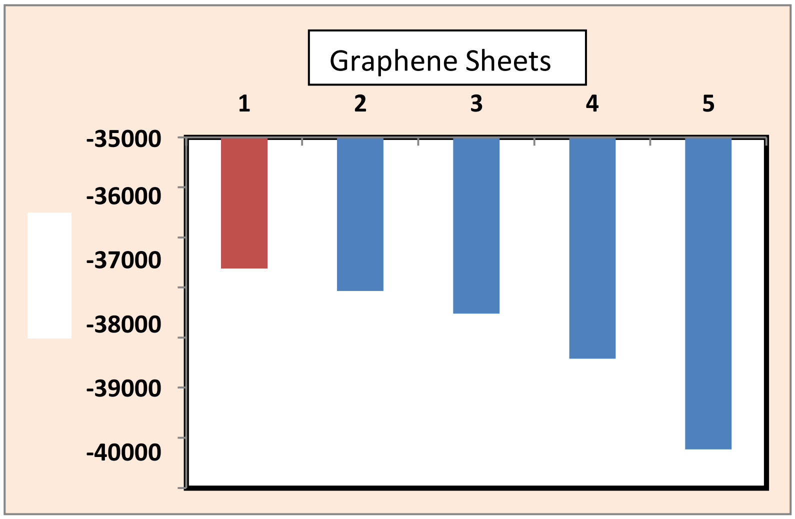


Figure (3.5): E_{total} in (eV) for Graphene Sheets

Figures (3.6) and (3.7) illustrated HOMO and LUMO energies of Graphene nanoribbons after adding. As seen, the HOMO's have differ behavior than the LUMO's. On the other side, the addition of Nitrogen atoms in the middle and terminal ends of phenylenes ring in the ribbons of(1, 2, 3and 4) changes the HOMO and LUMO energies, but the effect of the addition on HOMO is more than on LUMO. These results reflect the linear combination of atomic orbitals in both carbon and hydrogen an atom according to the basis sets that describe the individual componentsin the structure to construct the molecular orbitals.

The result of E_g in figure 3.8 illustrated that is the variation of E_g for the (1 and 2) in comparison with E_g for the (3 and 4). E_g for ribbon 3 was increased with adding the Nitrogen atoms in ribbon 4 , while for the others, shown E_g decreased with adding Nitrogen atoms ,E_g decreased from (0.97034 eV) for the ribbon 1 to (0.57796 eV) for ribbon 2 , and the E_g decreased with increasing the width of the ribbon, and therefore, increasing the number of added atoms in the ribbon, as shown in figure

3.8 . These global results gave molecular electronics important . 3-D shapes of HOMO and LUMO of GRs after adding are drowning in figure 3.9. The distribution of HOMO and LUMO calculated according to the total self-consistent field density calculations.

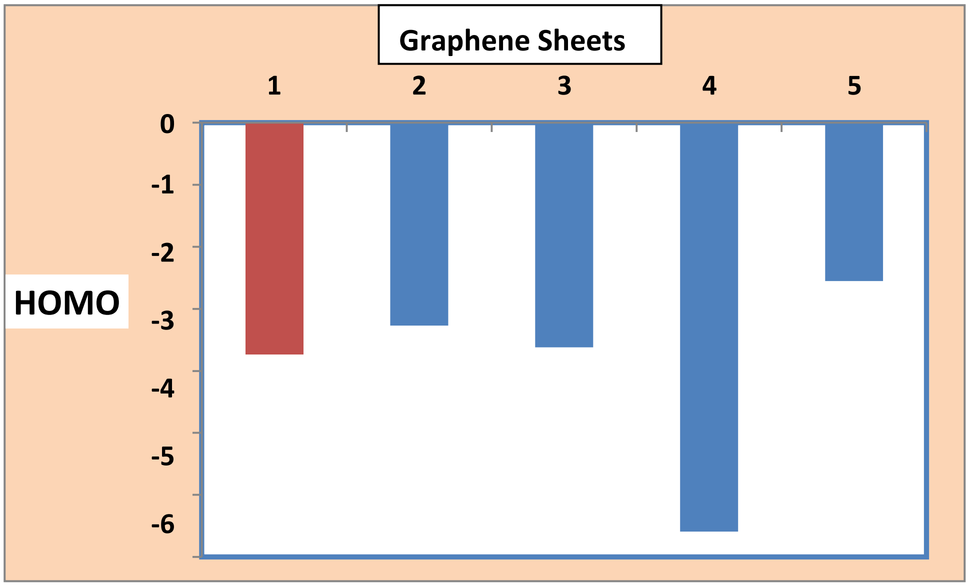


Figure (3.6): HOMO in (eV) for Graphene ribbons

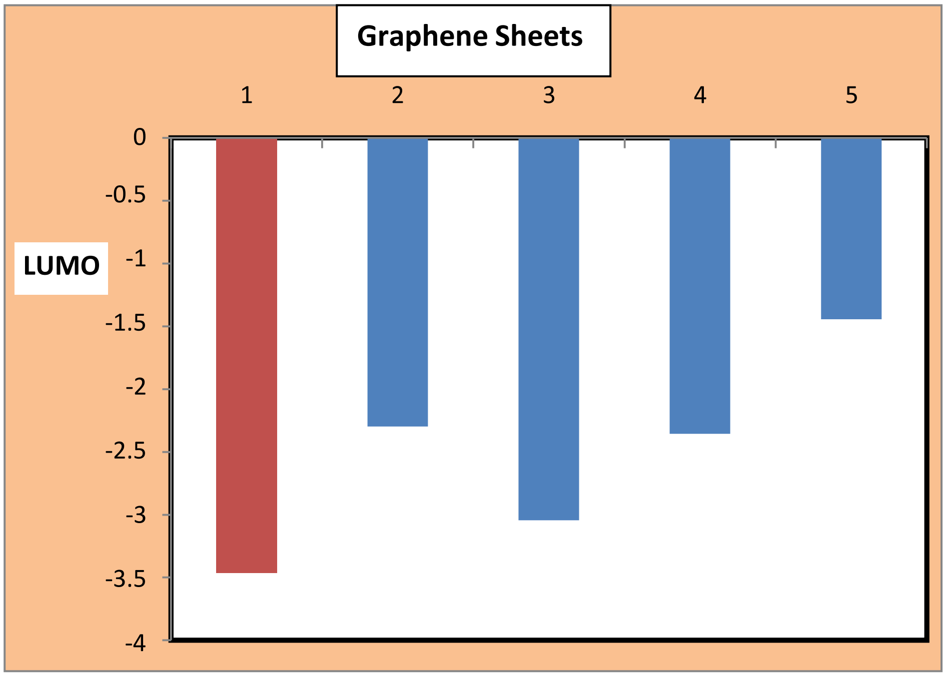


Figure (3.7): LOMO in (eV) for Graphene ribbons

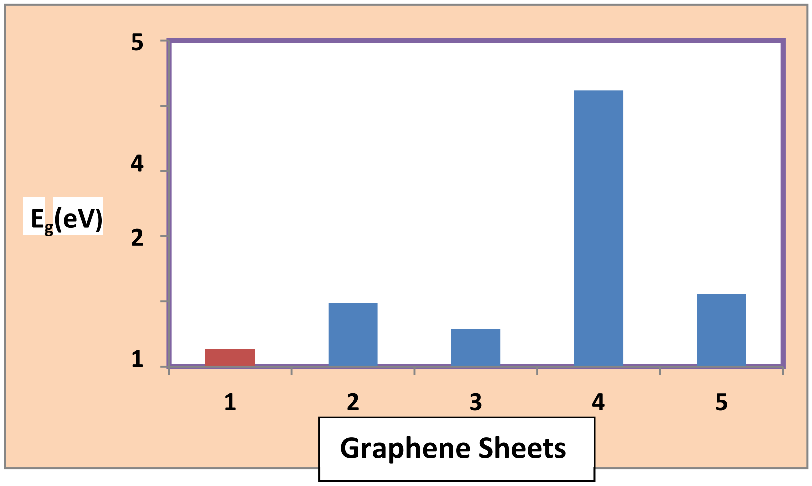
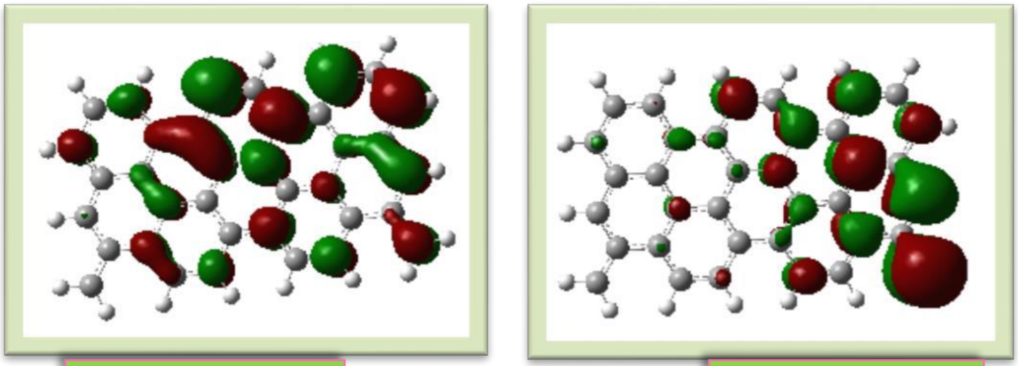


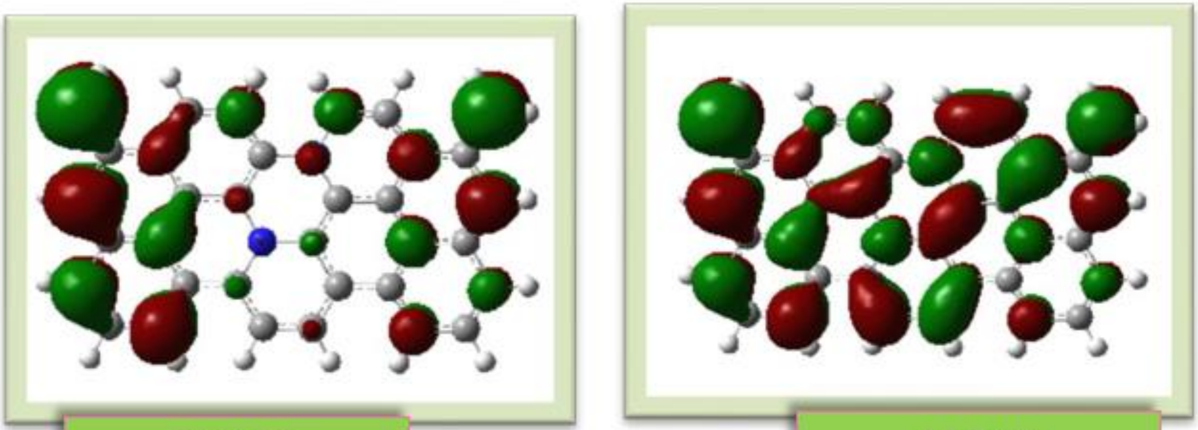
Figure (3.8): E_g in eV of the Graphene ribbons



HOMO

LUMO

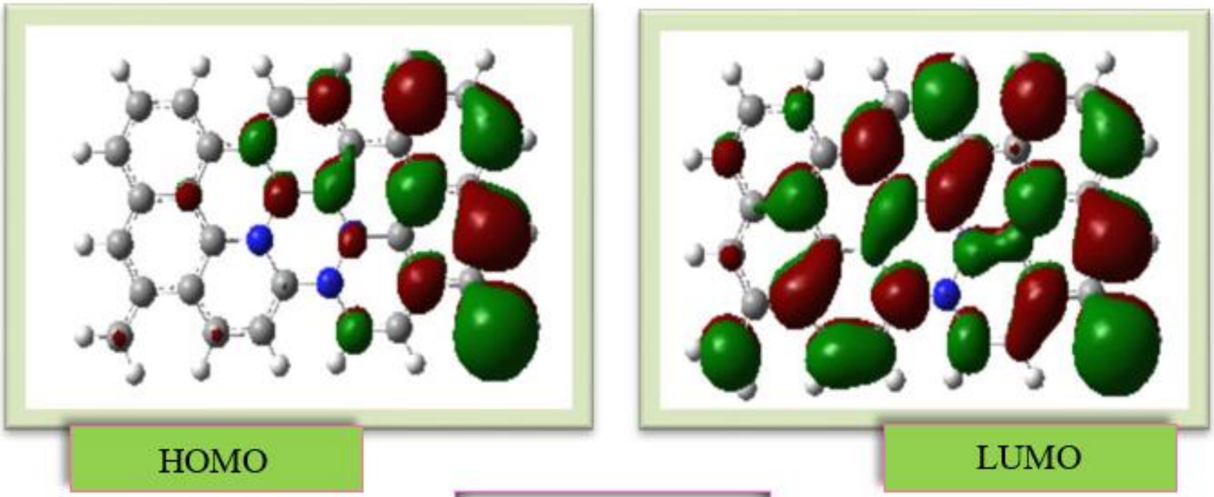
Ribbon 1



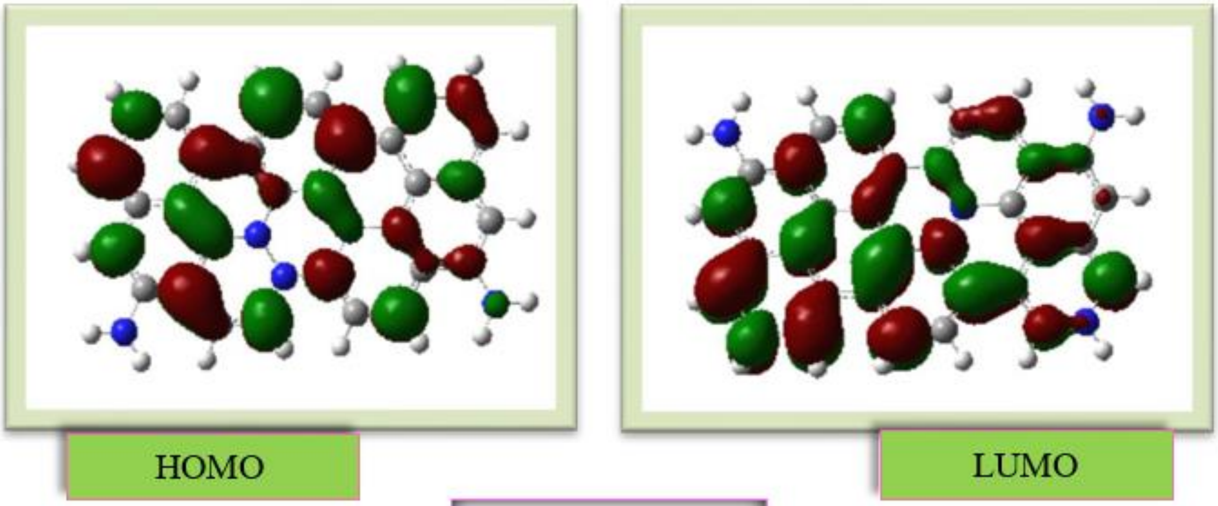
HOMO

LUMO

Ribbon 2



Ribbon 3



Ribbon 4

Figure (3.9): The 3-D shapes of HOMO and LUMO distribution of the Ribbons.

Conclusions

In this research the hybrid functional B3LYP with 6-31G basis sets under the theoretical methodology density functional theory has been concerned. The energetic features has been determined in order to employthe most popular called the koopman's theorem to identify the influencedfactors of ionization energy IE and electron affinity EA, and then investigating some important electronic properties, such aselectrochemical hardness H, electronic softness S. In addition, the electronic states (HOMO and LUMO) energies and energy gap for pure and doped graphene nanoribbons .

From the results, we can conclude the Doped graphene nanoribbons were designed here through replacingN_2 atoms in place of Carbon atoms in the terminal ends of ribbonin the pure sheet. The DFT calculations presented good result of total energies of all studied systems calculated from the summationof the total energies of the components for each structure .The totalenergy is decreasing with increasing the number of N_2 atoms to the ribbons, the electronic states HOMO and LUMO and have small energy gap compared with pure sheet that refer to ability to translation electrons cross energy band. Good relax done for the pure, the geometrical parameters (bond lengths) for pure calculated from DFT in current study have been found in good agreement with experimental data. Replacing the (C) atoms by N_2 atoms in the nanoribbons leads to a few reducing in the energy gap, this due to the linear combination of atomic orbitals of different atoms to construct the molecular orbitals. IE, EA of the pure sheet with N_2 atoms are greater than that of pure sheet without N_2 atoms in the terminal ends of the ribbons, while doping these ribbons in the N_2 atoms the property of IE and EA have high value compared with stander ribbons. Generally,new structures were constructed in this work with new various electronic properties. All the pure and doped graphene sheets have low electrochemical hardness H and high electronic softness S.High electronic softness is the main future as a sign for that band gap of the structure goes to be rather soft.

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