Synergy: Cross-Disciplinary Journal of Digital Investigation
(ISSN 2995-4827) VOLUME 02 ISSUE 9, 2024

THE INFLUENCE OF ADDING ALUMINUM ATOMS ON PROPERTIES OF GRAPHENE SHEETS USING DFT

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Abstract:

The structural and electrical characteristics of a pure graphene sheet as well as the results of varying the quantity of aluminum (Al) atoms added are the main theoretical subjects of this work. The pure graphene structures were designed using the Gauss View 5.0.8 software. The Gaussian 09 package of programs' hybrid functional B3LYP-DFT was used to relax these structures. Total energy (E_T), the energy gap (E_g), and the highest occupied and lowest unoccupied molecular orbital (HOMO) and LUMO energies were all computed. The electronic characteristics of the pure graphene sheet are effectively affected by the addition of Al atoms.

Keywords: Hybrid functional, Doping Graphene, Highest Occupied Molecular Orbital.

Introduction

The type of graphite known as graphene was first identified in 1962 by Hanns-Peter Boehm [1,2]. It can be regarded as a polycyclic aromatic hydrocarbon that is (infinitely) alternant (having just six carbon rings). Only when describing the responses, structural relationships, or other characteristics of individual layers should the word graphene be used [3,4]. A strong method for changing the characteristics of materials that resemble graphene is doping. By adjusting the doping settings, these materials' electrical characteristics can be customized [5].

Aluminum is a very important consumer metal. Its alloys are utilized in foil, cans of beverages, kitchen and food processing tools, electrical and architectural uses, and as the structural material for boats, airplanes, and other types of transportation [6]. In a variety of chemical and atmospheric conditions, numerous aluminum alloys demonstrate remarkable resistance to corrosion because of their naturally existing tenacious surface oxide film (Al2O3). Its resistance to oxidation and corrosion is essential for use in transportation and architecture. Aluminum is a superior electrical conductor compared to copper when considering weight and cost equally [7,8]. Because of its strong heat conductivity, it can be used in radiators and cooking utensils. Its low density makes it useful for industrial applications.

Aluminum is a fine silvery metal that conducts heat and electricity well and has a very low density. As was previously noted, air exposure causes aluminum's surface to produce oxides. Because of its large mass and ability to generate a thin, hard layer of aluminum oxide when exposed to air, aluminum has "self-protection" against erosion [9]. This layer sticks to the metal and keeps it from oxidizing further. Given the bulk of both components, its connectivity—which is double that of copper—allows it to be utilized in electrical cables, allowing aluminum wires to have a bigger diameter than copper wires. Its 39% greater expansion and contraction under the same heat as copper makes it a limited choice for electrical wire. Cans come in a variety of shapes and sizes, and thin coatings of aluminum are now utilized to package groceries, medications, and other home equipment [10]. Because aluminum hardens as temperature drops, alloys made of aluminum are also used to produce cans and other containers to store liquids at very low temperatures, such as nitrogen, argon, and oxygen [9,11].

Theoretical Parts

The most effective and promising method for calculating the electrical structure of matter at the moment is the density functional theory, or DFT. The electron thickness is a vital part of the density functional theory, which in its unique plan gives the ground state highlights of a system[12]. Various sub-atomic highlights, including sub-atomic designs, molecular frequencies, atomization and ionization energies, electric and attractive properties, and response pathways, are anticipated by DFT. Regardless of the system's electron count, it only depends on three coordinates, thus [13]:

$$N = \int \rho(\vec{r}) d\vec{r} \ldots\ldots\ldots (1)$$

The ground state energy is essential to DFT concepts, and the electron density is the only factor that can determine any other ground state electronic property. Moreover, given the lowest possible total energy, the system's precise ground state matches the electronic density[12].

Results and Discussion

The Nano Tube Modular program involves the design of zigzag graphene sheets and calculates their attributes. Gaussian View 5.0 was used to build each of these structures, and Gaussian 09 was used to analyze the data using basis set (6-31G) at (B3LYP).One ,two, four, or eight Al atoms are added to the pure graphene sheet to create the pure structure with properties. The length and types of bonds for pure sheets are described in Table (1). The range of bonds for (C-C), (C=C), (C,−.C), and (C-H) are, respectively, (1.45478–1.47808) Å, (1.34793–1.38478) Å, (1.39168–1.44396) Å, and (1.08155–1.08633) Å. The geometrical structure of the sheet is described in Figure (1).Table (2) provided an illustration of how their properties were calculated in electron volts (eV). Figure (2) illustrates how each sheet's overall energy is reduced when hydrogen atoms are present at the terminal ends of the phenylene rings. Between the structures GR2 and GR3, there is almost the same energy difference as there is between GR1 and GR4. The HOMO and LUMO energies of graphene sheets upon addition were shown in Figures (3) and (4). It is evident that the HOMOs behave differently from the LUMOs. Conversely, the HOMO and LUMO energies are altered by the addition of aluminum atoms to the middle and terminal ends of the phenylene ring in the sheets of GR1, GR2, GR3, and GR4. However, the effect of the addition is greater on HOMO than on LUMO. Based on the basis sets describing the constituent parts of the structure to build the molecular orbitals, these results show the linear combination of atomic orbitals in both the carbon and hydrogen atoms. Two observations can be made regarding the result of Eg in figure (5). The first is the variance of Eg for the GR1 and GR4 in relation to Eg for the GR2 and GR3. When aluminum atoms were added to structure GR4, Eg increased for structure GR3, but Eg declined for the other structures, going from (2.50722 eV) for GR1 to (0.28353 eV) for GR2. The second observation is that when the width of the sheets increased, the number of additional atoms in the ribbon also increased, causing the Eg to decrease. These worldwide findings made molecular electronics significant. Figures 9 and 10 show the 3-D forms of the HOMO and LUMO of GRs

before and after addition, respectively, and are identical. The HOMO and LUMO distributions were computed using the entire self-consistent field density computations. It is evident from Table 3.7 that the ionization energy (IE) of GRs in the GR2 is lower than that of the GR1 .This suggests that, in contrast to GR4 and GR5, GR2 and GR1 require less energy to donate electrons and turn into cations. Conversely, broadening the sheets' width. The structures (GR2, GR3, GR4, and GR5) also have greater electron affinity values (EA). The outcomes of IE and EA for GRs following the addition of aluminum atoms are shown in Figures 3.9 and 3.10, respectively.

Table (1): Display the stander sheet's bond kinds and lengths.

Bond	Values Å
C⁅C	1.44396
C-H	1.08633
C=C	1.38478
C-C	1.47808

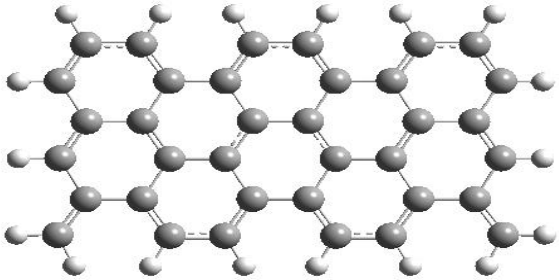
Graphene Sheet	Structure
Pure	

Fig (1): The geometrical structure of a pure graphene sheet.

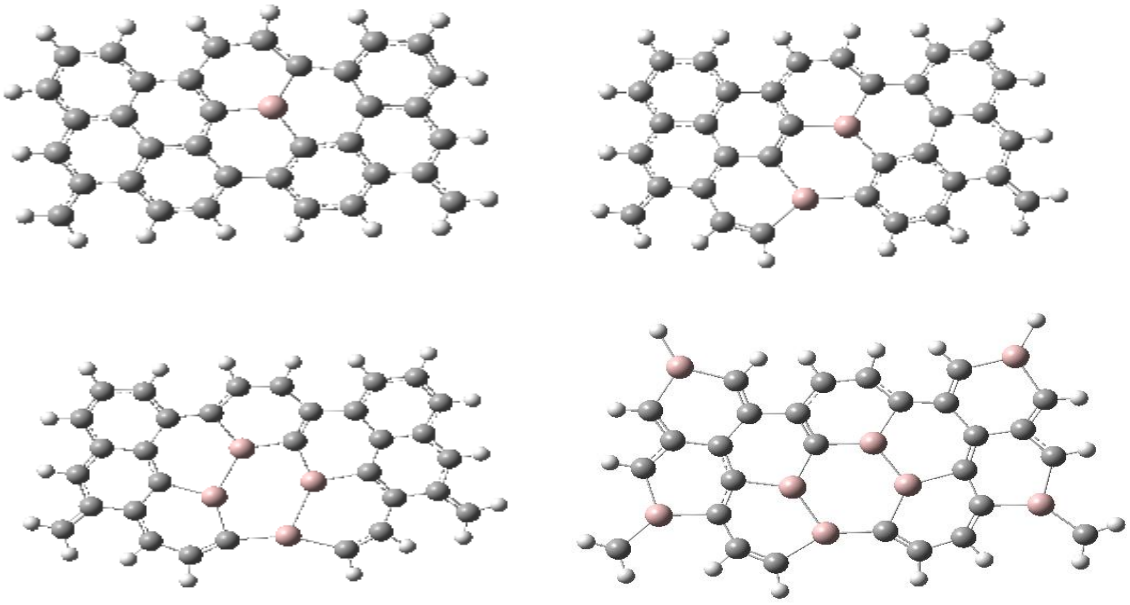


Fig (2): Relaxation structures for doped sheets under study.

Table (2): Electronic proprieties of the Pure and Doped Graphene Sheet**.**

Pure and Doped Graphene Sheet	Etotal(eV)	EHOMO(eV)	ELUMO(eV)	E_g(eV)	IE (eV)	EA (eV)
Pure	**-37616.3**	**-3.73661**	**-3.46287**	**0.273743**	**3.73661**	**3.46287**
GR1	**-43172.3**	**-4.85553**	**-2.34831**	**2.50722**	**4.85553**	**2.34831**
GR2	**-48731.4**	**-3.74042**	**-3.45689**	**0.28353**	**3.74042**	**3.45689**
GR3	**-59845.8**	**-4.29743**	**-3.64165**	**0.65578**	**4.29743**	**3.64165**
GR4	**-82082.2**	**-7.1954**	**-2.64899**	**4.54641**	**7.1954**	**2.64899**

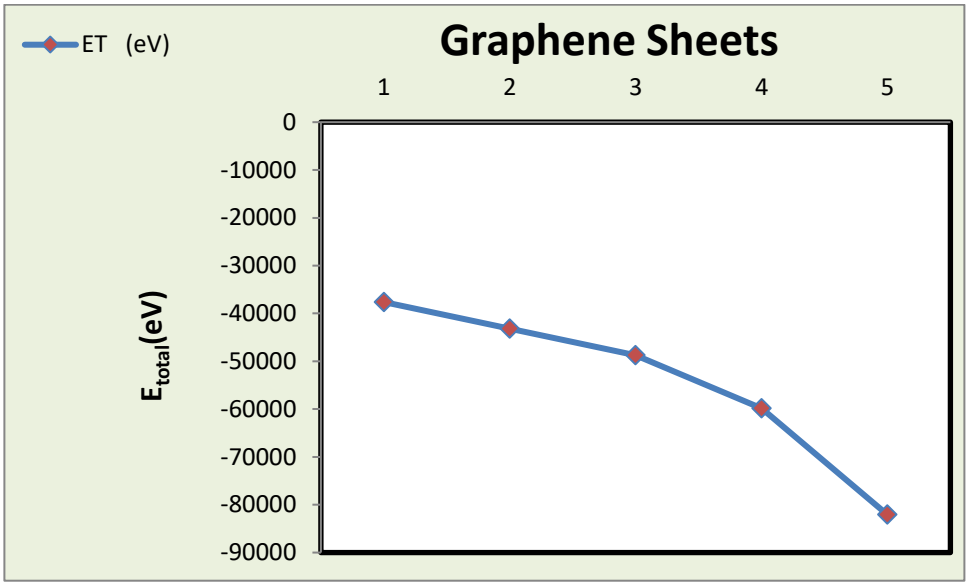


Fig (3): Etotal in (eV) for Graphene Sheets

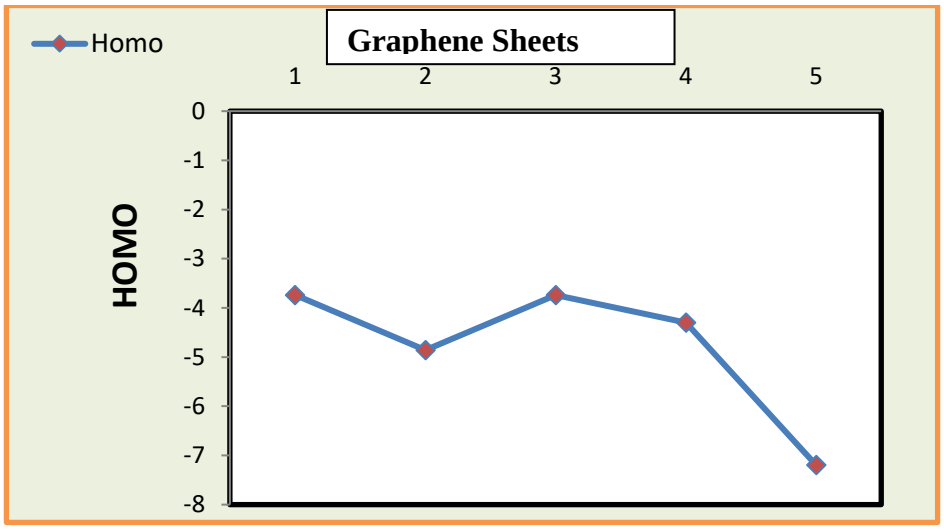


Fig (4): HOMO in (eV) for Graphene Sheets

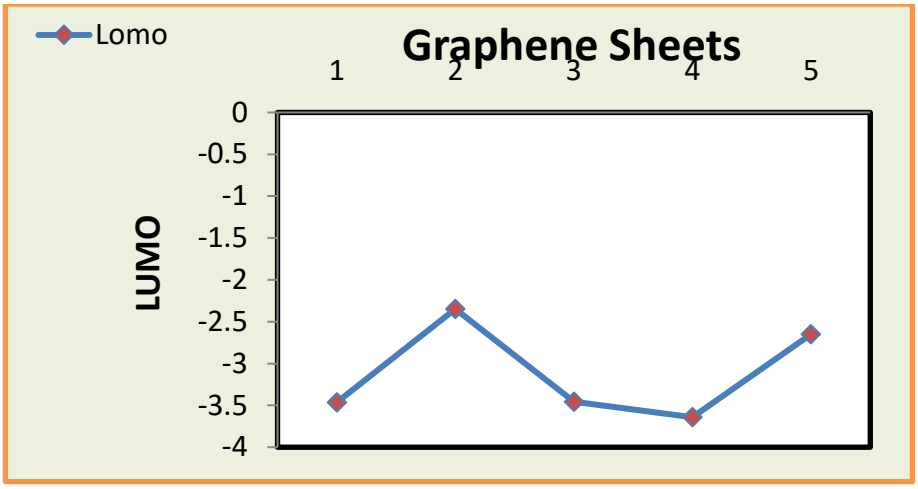


Fig (5): LOMO in (eV) for Graphene Sheet

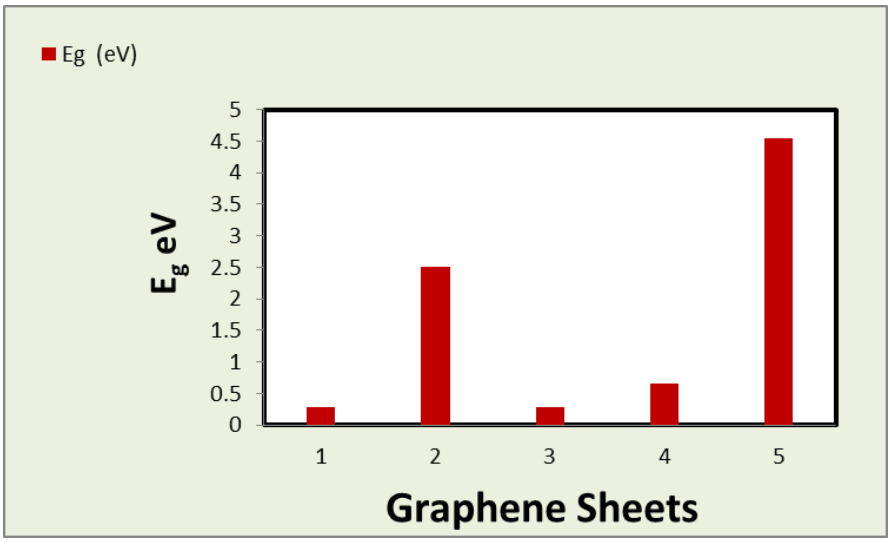


Fig (6): E_g in eV of the Graphene Sheet

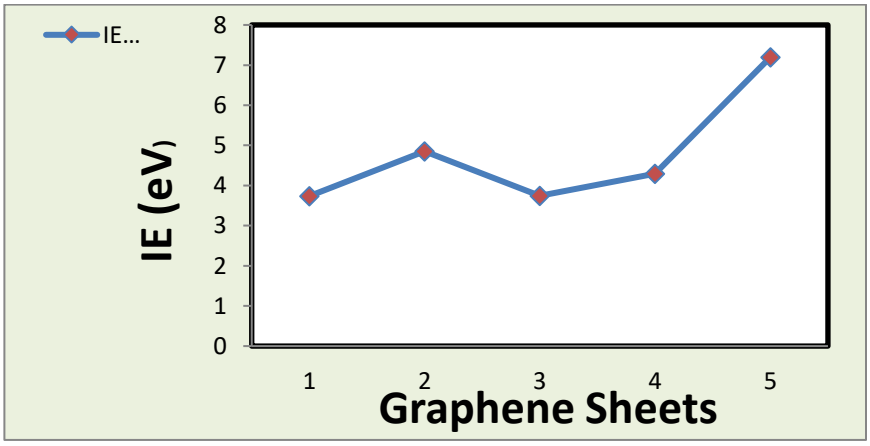


Figure (7): The IE of Graphene Sheets.

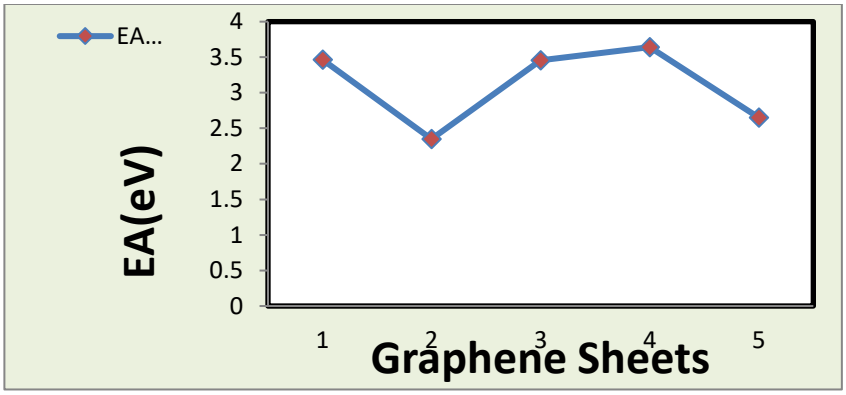


Figure (8): The EA of the Graphene Sheets.

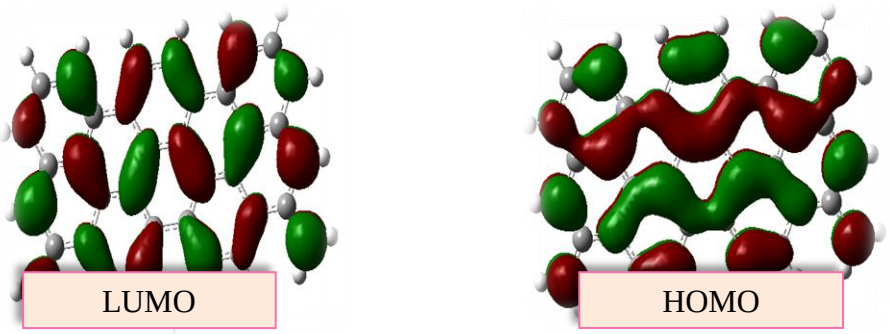


Figure (9): The 3-D shapes of HOMO and LUMO distribution of Pure Graphene Sheet GR1.

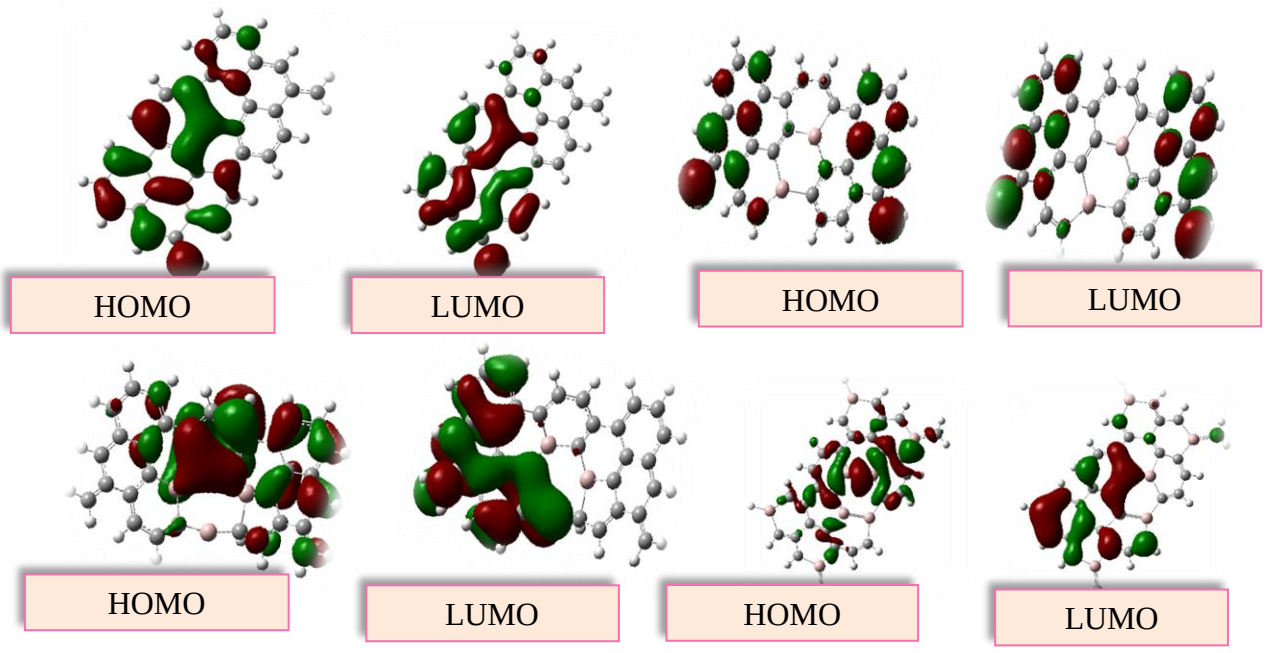


Figure (10): The 3-D shapes of HOMO and LUMO distribution of the GNRs for GR2,GR3, GR4 and GR5 respectively.

Conclusions

Density functional theory has been the focus of this investigation. DFTs rely on the energy of the ground state. To assess the accuracy of the results, use a premise set (6-31G) at capability (B3LYP) for an assortment of functions that make sense of a particle's orbital construction. Here, carbon particles in the terminal finishes of unadulterated sheets were traded out for (Al) molecules to make

doped graphene sheets. At the point when the all-out energies of the parts for each design are added up, the DFT presents the outcome, which is in concurrence with the consequences of a literature study [13, 14]. This outcomes in the all-out energies of all examined frameworks being assessed. The electronic states have a little energy hole contrasted with unadulterated sheets, which alludes to the capacity to interpret electrons across energy groups. The geometrical parameters (bond lengths) for unadulterated determined from DFT in this study have been viewed as in concurrence with exploratory information. The complete energy diminishes as the quantity of (Al) particles added to the sheet increments. The energy gap is slightly reduced when (Al) atoms are added to the sheets in place of (C) atoms. This is because the molecular orbitals are constructed by linearly combining the atomic orbitals of distinct atoms.

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