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Investigation Effect of Aluminum Atom on the structural, Electronic and Optical Properties of Graphene Nanomaterials using DFT

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Abstract:- In the two past decade graphene consider on of the important nanomaterials because it is having high surface area and unique properties like hardness and conductivity. In the present study structural, electronic and optical properties were carried by density function theory (DFT) calculation. The B3LYP hybrid function and 6-31G basis set were used to explain the exchange process. The geometrical calculation shows that the bond length between C-C, C=C, C-H and C-Al were agreement with experimental results. The Aluminum (Al) atom was effected on the surface nature, from the results we can see the defected was appeared on the surface of graphene nanostructure. Band gap calculation show that the pure graphene materials have band gap is 2.533 eV, by adding Al atom it reduces to 1.556 eV, in other hand we can conclude doping graphene materials by Al atom enhance the conductivity of the system. UV-Visible calculations show that pure graphene materials absorb at 522 nm, by adding Al atom, it shifts to red region of electromagnetic radiation. FT-IR calculation show that all carbon groups in stretching and bending mode were appeared in the pure graphene materials, in addition the Al-C carbon groups were appeared in the Al-graphene system. From above results conclude that Al atom was had direct effect on the structural, electronic and optical properties of graphene materials.

Keyword:- *Graphene, DFT, UV-Visible, FT-IR, Energy Gap.*

I. INTRODUCTION

A single layer of graphite known as graphene is composed of sp2 hybrid carbon atoms arranged in a honeycomb lattice. It consists of two interpenetrating triangular sub-lattices, and serves as the fundamental building block for carbon allotropes with other dimensions, such as fullerenes and carbon nanotubes[1]. A two-dimensional linked carbon sheet with superior surface to volume fraction, minimum electrical noise, and amazing transport qualities make up graphene, a fantastic material[2]. In addition to its distinctive two-dimensional structure and special chemical features, such as exceptional electrical, optical, and mechanical properties, graphene offers greater efficiency. Graphene offers a wide range of applications due to its exceptional features, including energy production, spintronics, and field effects transistors (FET)[3]. It has also been demonstrated that graphene may have theoretical and experimental applications in detecting molecules. Due to its small size and high surface area, graphene may be used as a new material for adsorption and desorption[4]. With its valence and conduction bands contacting in a Brillion zone corner, graphene is a zero band gap semiconductor and has what are known as Dirac points[5]. The capacity to open a tunable band gap is necessary for the development of graphene-based electronics. Several methods have been devised to construct high-performance graphene devices by engineering their band gaps to enhance their semiconducting capabilities[6].

II. GRAPHENE DOPED MECHANISM.

More research has focused on specific features since the discovery of graphene in 2004[7], including capacitors, lithium-ion batteries, gas sensors, and spintronic devices. Due to its strong thermal and electrical conductivity, gas sensor mechanisms employ it extensively[8]. Due to the sp2 bonding between the carbon atoms in the graphene plane sheet, pure graphene is relatively chemically inert, which poses a significant obstacle to its potential use in gas-based sensors[9]. Due to its high specific surface area, it can transfer charges to external gas molecules that have been adsorbed[10]. Graphene, however, exhibits weak physical adsorption of the majority of gas molecules, according to numerous theoretical and experimental studies[11]. Thus, a variety of processes, including defect vacancies and doped graphene with metal atoms, were used by researchers to tackle this problem[12]. Electrical conductivity, chemical reactivity, and important structural and electronic features were produced by graphene doped with metal atoms during the process of adsorption to detect tiny gas molecules[13]. It is important to note that doping graphene with metallic atoms causes alterations without causing even one atom of the material to be damaged[14]. Many studies demonstrate that adding a flaw or doped metallic atom to graphene would change the strength of the charge transfer between it and the gas molecules it has adsorbed, as well as increase the

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sensitivity and selectivity of gas-based sensors[15]. Gas sensing was a significant environmental challenge for the molecules of hazardous poisonous gases. One of these gases was the monooxide (CO) molecule, which has received extensive attention due to its negative effects on human health and its significance as the primary air pollution culprit[16]. CO adsorption on nanotube surfaces, including those made of boron-nitride, aluminum-nitride, and aluminum-phosphide, as well as other III-V group of element table structures[17]. Results of a prior study that altered the sensitivity and selectivity of copper, nickel, platinum, and the III-V group to dope them[18]. According to research by other scientists, metallic atoms doped into graphene increase its chemical sensitivity to molecules of carbon monoxide (CO), sulfur dioxide (SO2), and ammonia (NH3).

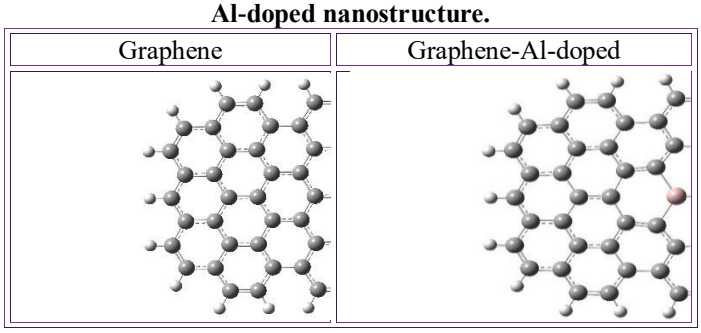
III. TOOLS AND METHODOLOGY.

In this study, nano tube modular is utilized to create graphene nano-ribbon structures with n=m=3 and tube lengths of 1 nm. For the display system, export the structure to the Gaussian 5.0 version. the input data is then exported to Gaussian 09. The bond length and atom-to-atom angle are structural features. The energy gap, ionization potential, and electron affinity are all examples of electronic properties. UV-visible and FT-IR spectra are involved in optical characteristics.

IV. GEOMETRICAL PROPERTIES FOR PURE AND AL-DOPED GRAPHENE MATERIALS.

Bond length and angle between atoms, two geometric properties computed for graphene nano-ribbon. The geometric structure for boron-nitride nanoribbon and pure graphene is shown in Figure (3-1). The values of bond length are in conformity with previous research[105] and are (1.4555), (1.3661), (1.4305), and (1.0859) for C-C, C=C, C=C (aromatic), and C-H. The specified angles for (C---C---C) and (C=C-H) are 120.232 and 119.922 degrees, respectively[19]. Bond lengths for the three carbon atoms that encircle the Al atom in an Al-doped nanoribbon range from 1.74183 to 1.76034. For C-C, C=C, C-C, and C-H, the corresponding bond lengths are (1.45008-1.51082), (1.37120-1.38314), (1.38829-1.44190), and (1.08360-1.08500), respectively. Al-C-C and C-C-Al have bond angles of (119.53093) and (113.38705) degrees, respectively[124]. For C-C-C, C=C-C, C-C-H, C=C-H, and C-C-C, the modified angles between the carbon atoms are (119.92835-128.96072), (113.40698-133.20658), (117.15782), (117.19586-121.04857), and (113.51606-121.00577), respectively[20]. Figure 1 represent the geometrical structure for pure and Al-doped graphene materials.

Fig 1. listed the geometrical structural for graphene and Al-doped nanostructure.



V. ELECTRONIC PROPERTIES.

Table (1) lists electronic Properties of Al doped graphene compared with pure graphene. According to the results for pure graphene, the system has less overall energy than an Al-doped system, which means that Al atoms make the system more stable. The molecular orbital energy of graphene materials is directly impacted by the alpha atom, shifting it to a lower energy level. Graphene and the Al-doped system are both semiconductors, according to energy gap calculations, however the Al-doped system has higher conductivity than the pure structure[21]. Ionization potential and electron affinity calculations reveal that pristine graphene has a high ability to designate an electron and become an anion.

Table 1. Listed the values of electronic properties for the systems under study.

System	Pure G.	Al-G.
E_T (a.u.)	-1916.0381	-2119.9411
HOMO (eV)	-4.7809	-8.0356
LUMO (eV)	-2.2471	-6.4797
E_g (eV)	2.533	1.556
IP (eV)	4.7809	8.0356
EA (eV)	2.2471	6.4797

VI. OPTICAL PROPERTIES

➢ ***UV-Visible***

With a basis set of 6-31G and a hybrid function of B3YLP, UV spectra are computed using TD-DFT. Calculating the optical properties of graphene and Al-doped nanoribbons was essential for finding see whether shifting were blue or red and for computing excitation energy. The results show that pure graphene ribbon absorbed in the visible spectrum, with the highest absorbed wavelength being equal to (525.2) nm and the excitation energy being equal to (2.36) eV[22]. UV-visible spectra of Al-G are shown in figure (4-2). UV spectra demonstrate that the doping mechanism changed the absorption wave length to the red, which is located at a wavelength of 1276.36 nm, which is higher than the absorption wave length of pure graphene, which is 533 nm. This finding demonstrates that an electron only needs a small amount of absorption energy to move from the LUMO level to the HOMO level[23]. Fig 2 illustrated UV-visible spectrum for the systems under study.

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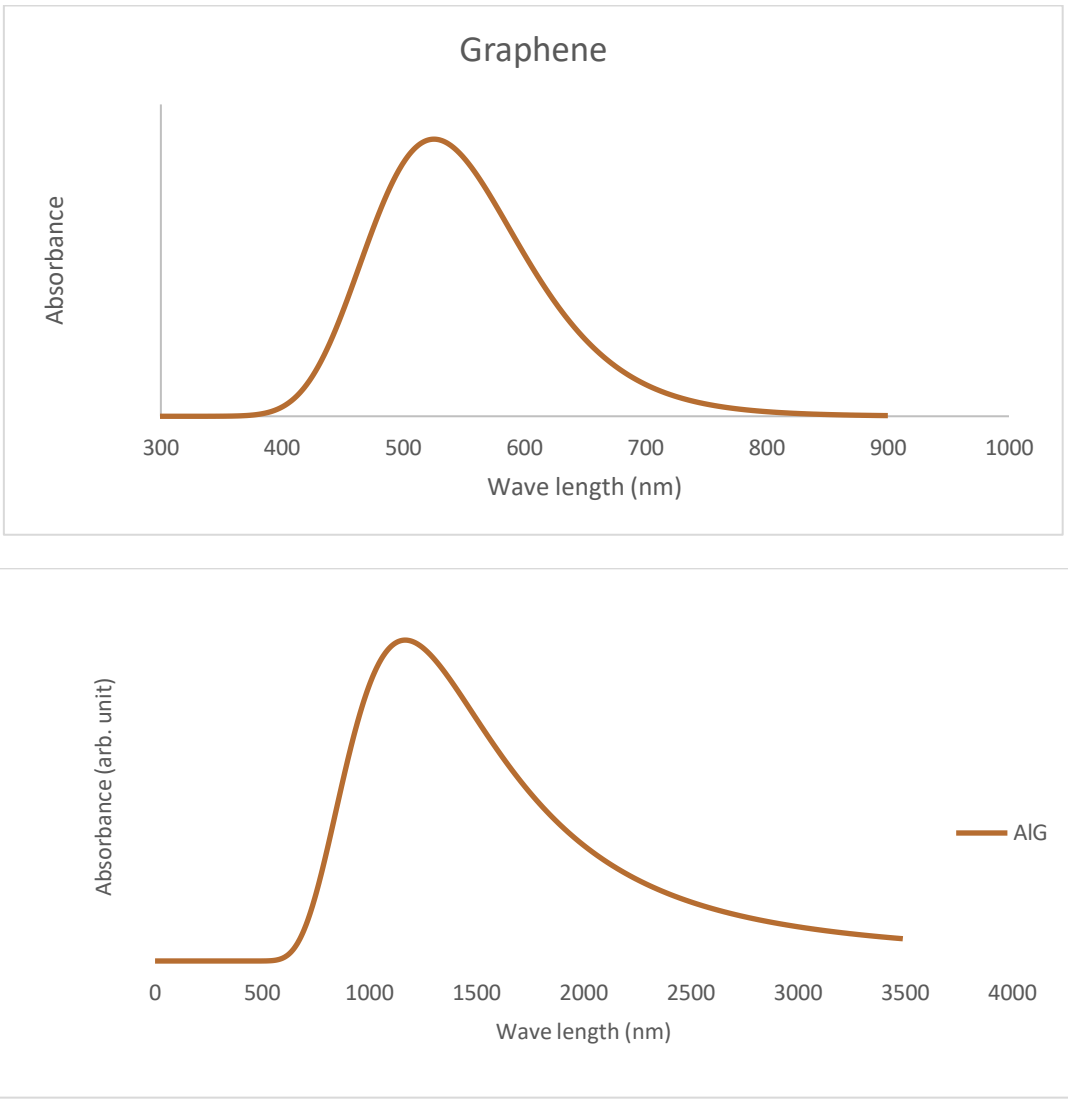

Fig 2. represents UV-Visible spectra of pure and Al doped graphene nanostructures.

➢ *FT-IR spectrum analysis.*

In this section Fourier Transformation- Infrared radiation (FT-IR) spectroscopic is studied to determine functional group for graphene and boron-nitride in pure case. The functional group of (C-C) appeared on a surface measuring 1600.18 cm-1 for pure graphene, (=C-H) appeared on a surface measuring 3186 cm-1 to represent an aromatic sp2 hybrid, and (C-H) sharp appeared on a surface measuring 928 cm-1 to bend with an alkene group[24]. The spectral characteristics will change if Al atoms are substituted for C atoms in the nanosystem. Adsorption system FT-IR spectra are shown in Figure (3). Al-C in starching mode appears at 1477 cm-1 for the AlG nanoribbon's spectrum new Al-C peak at 889 cm-1. AlG nano-fundamental ribbon's bonds, (C-C), (C=C), and (C-H), are visible at peaks at 1230 cm-1 stretching mode, 1512 cm-1 stretching mode, and 3209 cm-1 skew-symmetric mode, respectively.

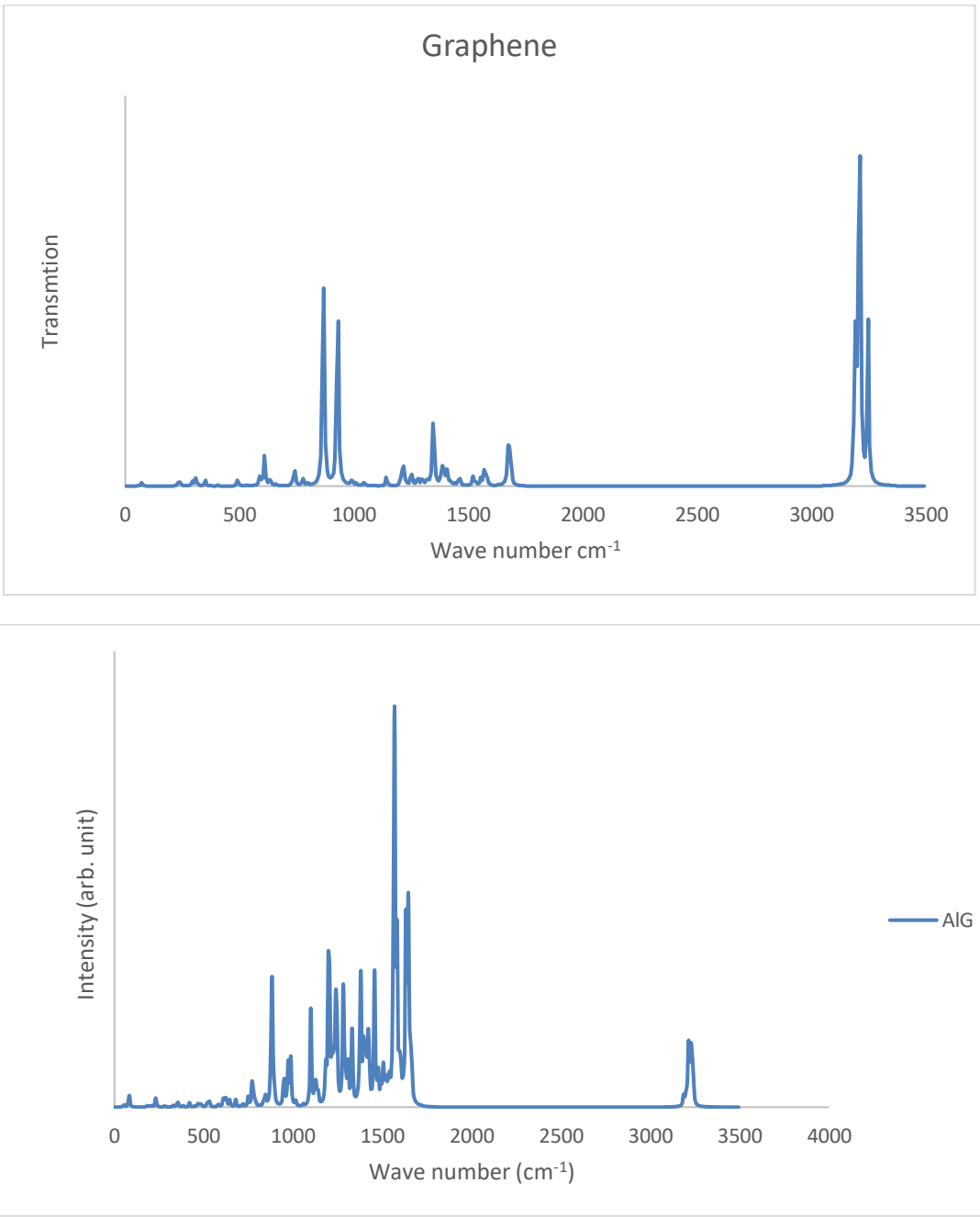

Fig 3. Illustrated FT-IR spectrum for pure and Al-doped nano structures.

VII. CONCLUSION

- DFT tool is useful method to computed ground state properties for 2D materials.
- Band gap calculation shows that an agreement between experimental and theoretical calculation.
- Al atom enhance the electrical conductivity of graphene nano structure.

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