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Study Adsorption Energy of CO Gas Molecule on the Surface of Pure Graphene Nano-Ribbon using DFT Calculation

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Abstract: In present study density function theory (DFT) was used to computed geometrical, electronic and optical properties for graphene nano-ribbon in absence and present gas molecule. Geometrical calculation show that graphene nano-ribbon has plane surface in absence and present gas molecule, bond length between C-C is 1.42Å. Electronic properties show that graphene nano-ribbon has semiconductor nature according to energy gap value. Adsorption calculation shows that chemical interaction occurs in distance near surface and decreased gradually when gas molecule become far from graphene nabo-ribbon surface. UV-Visible spectrum changed only in chemical adsorption and this clear in distance 1, 1.5 and 2 between gas molecule and surface.

I. INTRODUCTION

Graphene is the name given to a single layer of graphite, made up of sp^2 hybrids carbon atoms arranged in honeycomb lattice, it consists of two interpenetrating triangular sub-lattice and is a basic building block for carbon allotropes of other dimensionalities similar to fullerenes and carbon nanotubes[1]. Graphene as a two-dimensional connected carbon sheet is an excellent material that has exceptional properties such as superior surface to volume fraction, little electrical noise and outstanding transport properties. Graphene has more superior efficiency in addition to its unique two-dimensional structure and has unique chemical properties such as outstanding electrical, optical and mechanical properties[2]. Due to its excellent properties, graphene has been commonly used in a number of ways, such as energy generation, spintronics and field effects transistor (FET)[2]. Graphene has also been proven to have possible uses in detection molecules, both experimental and theoretical. Graphene may be chosen as a novel material for adsorption and desorption due to its low dimensions and wide surface area process. Graphene is a zero band gap semiconductor with its valence and conduction bands touching in corner of the Brillion zone in called Dirac points[3]. Development of graphene based electronics depends on ability to open a tunable band gap, various approaches have been developed to fabricate high-performance graphene device by engineering their band gaps so as to improve their semiconducting properties[4]. Present study aim to an investigation strength of adsorption energy for CO gas molecule at different distance from surface related to pure graphene nano-ribbon.

II. COMPUTATIONAL DETAILS

In present study density function theory was used to estimate geometrical and electronic properties of pure and doped graphene nano-ribbon at basis set 6-31G with hybrid function B3LYP. Geometrical properties involve bond length and angle between atoms. Electronic properties split to molecular orbital energy, energy gap and adsorption energy. Nanotube modular software was used to build nano structure. Gaussian view 5.0 software was used to visualized and computation properties under study[5].

III. GEOMETRICAL PROPERTIES AND ENERGETIC FOR PURE GRAPHENE

Geometrical characteristics summarized on bond length and angle between atoms computed for graphene nano-ribbon when toxic gas molecule absence. Figure (1) lists the geometry structure for pure graphene. Bond length for C-C, C=C, C=C (aromatic) and C-H are (1.4555), (1.3661), (1.4305) and (1.0859) Å values of bond length are agreements with past study. Angles between atoms listed for (C--C--C) and (C=C-H) are 120.232 and 119.922 degree[6]. Total energy, molecular orbitals (HOMO and LUMO), energy gap, ionization potential and electron affinity summarized by the listed Table (1). The result shows that the graphene nano-ribbon was semiconductor material and boron-nitride was insulator material.

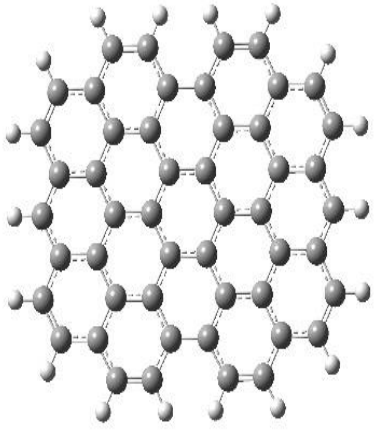

Fig. 1: lists the geometry structure for pure graphene

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Property	Graphene nano-ribbon
Et (a.u.)	-1916.0381
HOMO (eV)	-4.780973
LUMO (eV)	-2.247084
Eg (eV)	2.533888
IP (eV)	4.780973
EA (eV)	2.247084

Table 1: properties for pure graphene and boron-nitride nano-ribbon

IV. ADSORPTION ENERGY FOR CO GAS MOLECULE ON SURFACE OF GRAPHENE NANO-RIBBON

First step determines full relaxation between gas molecule and graphene nano-ribbon and determine minimum energy of stability, also type of adsorption. Second step change adsorption distance between gas molecule and the surface of graphene nano-ribbon[7]. DFT calculation show that relaxation distance between gas molecule and the surface 3.88Å and adsorption energy was -0.05 eV, also type of interaction is physical[8]. Now, the study effect changes distance on adsorption energy to enhance the sensitivity of graphene nano-ribbon for these gases.For CO gas molecule adsorption distance that far from the surface,indicate that graphene sensitive to gas molecule but in a small amount of energy transfer between them this clear for distance 4 to 3 and type of adsorption was physical[9]. Distance 2.5 to 1 Å adsorption energy increasing and nano system began sense to a gas molecule. Increasing in adsorption energy led to the formed bond between C atom related to graphene ribbon and C atom for gas molecule[10]. Bonding led to chemical adsorption that rising high adsorption energy. Energy absolute value increasing from 0.922 to 34.0385 eV. Figure (2) show curve of adsorption energy and distance between CO and surface of graphene nano-ribbon and split-step equal 0.5 Å.

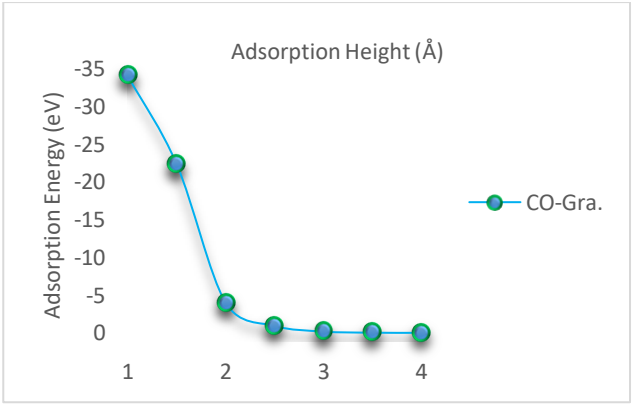

Fig. 2: show curve of adsorption energy and distance between CO and surface of graphene nano-ribbon and split-step equal 0.5 Å.

V. MOLECULAR ORBITALS AND ENERGY GAP

Higher Occupation Molecular Orbitals (HOMO), Lower Unoccuption Molecular Orbitals (LUMO) and Energy Gap (E_g) are important parameters to determine ability of electrons transition and type of materials classification (Conductor, Semiconductor and Insulator)[11]. First energy gap for stander ribbon without gas interaction on surface, energy gap for graphene ribbon is 2.533 eV is semiconductor materials. For pure graphene nano-ribbon HOMO & LUMO was distribution around C-C bonding. Distribution of molecular orbital of it was symmetry[12]. Table (2) represent HOMO, LUMO and energy gap for adsorption process.

D (Å)	HOMO	LUMO	Eg
1	-4.1311	-2.5425	1.588
1.5	-4.2468	-2.6911	1.555
2	-4.8533	-2.3480	2.505
2.5	-4.8171	-2.2868	2.530
3	-4.7978	-2.2653	2.532
3.5	-4.7913	-2.2582	2.533
4	-4.7899	-2.2566	2.533

Table 2: represent electronic state and energy gap for interaction system in eV unit.

The HOMO is more essential orbital on the charge transfer consequently always to graphene. Because mainly it located on the atom of gas molecule, the charge transfer is largest when atom of gases are closed to surface. Results indicate that for distance near surface of graphene nano-ribbon molecular orbitals overlap gas molecule and scattering region of the surface because high adsorption mechanism, in other hand high amount of electrons transfer from graphene nano-ribbon to gas molecule[13]. Also increasing distance between them all molecular orbitals energy fixed on pure state of graphene nano-ribbon. distribution of HOMO and LUMO for these distances remain at pristine graphene nano-ribbon this mean no hybridizing also weak interaction between them. Energy gaps depends on difference energy between HOMO and LUMO value. Results in Table (2) show that energy gap decreased when interaction increasing when gas molecule near surface and Van Der Waals occur. Also result indicate when energy gap decreased during chemical adsorption the graphene nano-ribbon have high stability. Result show that also for distance far from the surface energy gap for adsorbed systems remain at pristine graphene nano-ribbon energy gap, in other hand decreasingin electron transport through band energy[14]. Figure (3) represent HOMO and LUMO distribution for adsorption systems.

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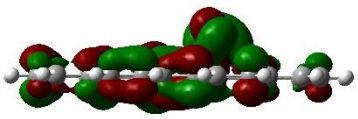
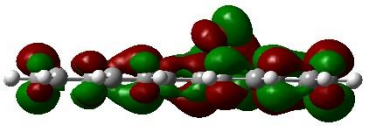
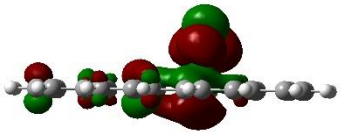
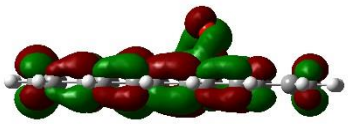
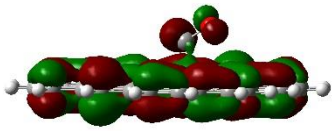
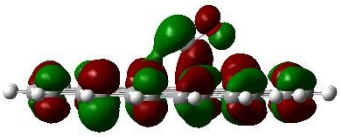
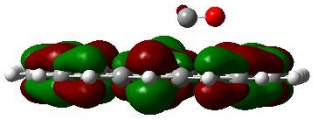
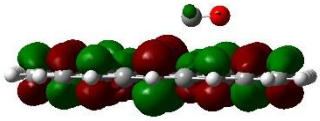
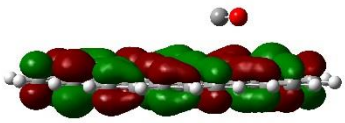
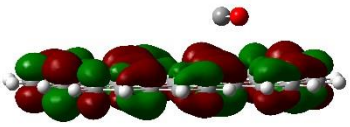
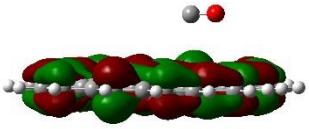
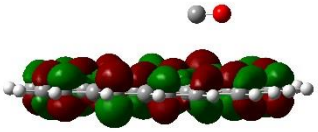
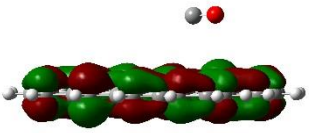
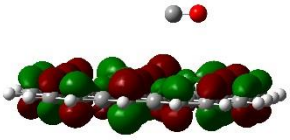
D (Å)	CO-HOMO	CO-LUMO
1		
1.5		
2		
2.5		
3		
3.5		
4		

Fig. 3: represents molecular orbital energy for interaction system

VI. UV-VISIBLE SPECTROSCOPIC

In this part of study effect of gas molecule on optical Properties for graphene nano-ribbon, determine type of shifting blue or red. Optical calculation is important part to determine type of shifting for adsorption gases on surface of graphene ribbon. TD-DFT method used to compute UV-Visible Properties at basis set 6-31G with hybrid function B3LYP. for pure graphene ribbon maximum absorbed wave length is equal (525.2) nm. Table (3) represent maximum wave length absorbed by adsorbed system. Result indicate that all UV-Visible spectra has a red shift. In chemical adsorption mechanism appear 2 and 3 transition state and this clear in distance 1 and 1.5 Å. Also results indicate when adsorption distance increase ability of interaction between gas molecule and surface decreased. The wave length of absorption decreased until fit on pure graphene nano-ribbon and this prove that interaction was vanishing[15].

D (Å)	λ-CO
1	562.84 756.2 1156.49
1.5	573.37 681
2	537.71
2.5	527
3	525.78
3.5	525.5
4	525.44

Table 3: represent maximum wave length absorbed by adsorbed system

VII. CONCLUSIONS

In present study investigation adsorption energy between gas molecule and surface of graphene nano-ribbon. Chemical adsorption effect directly on electronic properties

such as energy gap, also distribution of charge density around surface. Physical adsorption doesn't appear any effect on nano-system.UV-Visible calculation show that's spectrum shifted to red reigon of electromagnetic radiation, only in chemical adsorption. Physical adsorption doesn't give any sign to change in spectrum.

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