University of Thi-Qar Journal of Science (UTJsci)
E-ISSN: 2709-0256, P-ISSN: 1991-8690, Vol. 11, No. 1, Jun. 2024

Theoretical Study of External Electric Field Effect on the Chemisorption of a Spherical Semiconducting Quantum-dot on Graphene

Marwa Q. Abd-AlHussien [1a] and H. K. Fadel*[2b]

[1,2]*Department of Physics, College of Education for Pure Sciences ,University of Basrah, Basra, Iraq*
[a] Email: aledany2012@mail.ru
[b*]Corresponding author: haider.qassim@uobasrah.edu.iq

Received: 2024-02-10, Revised: 2024-02-23, Accepted: 2024-02-25, Published: 2024-06-01

***Abstract*—In This study, we modified the Anderson-Newns model for atomic chemisorption to be suitable for the chemisorption of a spherical semiconducting quantum-dot on a monolayer pure perfect graphene.**

A mathematical expression was used to calculate the occupation numbers for the two levels of the quantum-dot as a function of the normal distance and the external electric field. Appropriate formulas for other chemisorption functions were used by taking into our account the effect of image shift, and a formula for hybridization energy as a function of distance only. The quantum-dot was considered a spherical shape, chooses the type of on-top adsorption on the graphene layer, also taken a fixed value for the correlation energy U to be spin independent and not dependent on distance.

At room temperature T=300 K, the occupation numbers and their corresponding energy levels were calculated by stabilizing all the parameters $\alpha, V_{\circ}, U, d_{\circ}, \varepsilon_{dot}$ and varying the strength of electric field individually by both positive and negative directions. The contribution of the negative electric field was more effective on quantum-dot chemisorbed on graphene.

***Keywords*—Chemisorption, Quantum Dots, Graphene, Quantum Dots Adsorption**

I. INTRODUCTION

Studying the adsorption of atomic particles on a solid surface is one of the necessary issues that paves the way for examining the desorption process. Desorption process is opposite to the adsorption process, i.e. it means removing adsorbed particle from a surface on which chemical process occur. Also, adsorption process differs from the absorption process, because the first one represents the adsorption of atomic species on the surface, while absorption process happens due to the easiest of penetration the surface and the entry of particles into the solid surface. Adsorption can be divided into two types depending on the nature of the bond between the adsorbed particle and the surface and the location of the adsorbed particle on the surface [1-3]: Physical adsorption (Physisorption). In this type of adsorption the Van Der Waals bond is the only bond where there is no redistribution of electronic charges neither on the adsorbed particle nor on the surface. For example, in physical adsorption of inert gases, the depth of the potential barrier is 0.2 eV at a temperature 300 K with an average residence time on the surface is about 10^{-8} sec [4]. The second type is the chemical adsorption(Chemisorption). In this type of adsorption, a bond that formed between the surface and the adsorbed particle is a strong chemical bond because of the redistribution and arrangement of the electronic charges, the nature of this bond either ionic or covalent bond. So, the chemical bond between the adsorbed particle and the surface is characterized by a depth of negative potential curve at distance closing to the surface. Chemisorption is considered as one of the most important procedures of studying the chemical reactions on the surface. In order to understand the theory of chemisorption, we will study how adsorption provides a clear explanation about the nature of the formed bonds and charge exchange in the adsorption region [5].

Quantum confinement in quantum-dot means restricting the movement of electrons and holes in all direction due to the electrostatic potential [6]. The dimensions of the quantum-dots are microscopically around 1nm, meaning they are very small leading to discrete energy levels and the density of states is a delta function. Adding (or removing) small numbers of atoms to (or from) the quantum-dots will affect the changes in the limits of the band gap due to the small size of quantum-dots and the effects of quantum confinement. It is also possible to change the geometry of the quantum-dot surface. Quantum-dots are considered a semiconductor because they are very close and related to the size and shape of the single crystal [7]. Quantum-dots are involved in many applications, including single electron transistors, light-emitting diodes, lasers, single-photon sources and second harmonic generation in quantum computing and the fields of medicine. Quantum-dots have intermediate properties between conductors and discrete atoms or molecules whose properties change as a function of both size and shape [8,9]. Carbon nanomaterials have attracted the attention because of their distinct and tunable electronic and structural properties [10,11]. The electrons and holes in graphene have a linear dispersion relation [12,13] and the charge carriers in graphene are homogeneous [14,15], so these properties has amazing

https://doi.org/10.32792/utq/utjsci/v11i1.1164

results such as (half integer) in the quantum Hall effect[16,17].

Nanoparticles may adsorbed on the surface of pure graphene on one of three different locations [18-20], they can be above the center of unit cell and called hollow (H) , above the C-C bond which called bridge (B)or on a carbon atom that called on top (T). Since graphene is a semiconductor with zero gap, so the band energy near the Fermi level is dispersed [21-23] Therefore, we can consider the electrons around the Fermi level to be two-dimensional massless Dirac fermions with replacing the speed of light c by the speed of Fermi level υ_F[24-26]. Understanding the effect of the electric field on the physical and chemical properties of 2D nanostructures is useful in the design of new electronic and optoelectronic devices. Many of these properties are described by the dielectric constant, which plays an important role in capacitance, conductivity, dielectric losses, and refractive index.

Through modern theoretical studies and the use of Density Functional Theory (DFT) calculations, including Van Der Waals interactions on graphene, the focus is on graphene due to its complementary physical and chemical properties and the increasing interest in the process of integrating it into the next generation of electronic devices and optoelectronics. Although the topic of nanotechnology is one of the most important priorities for researchers at this time, in spite of the a lot of studies that have been done on the chemisorption of atoms or molecules on the graphene, no one have discussed the effect of the electric field on the adsorption of quantum-dots on graphene, but there are many important articles and studies on the chemisorption of atoms or molecules on the graphene.

II. THEORY

When a charged particle approaches a metal surface, the electronic response leads to a polarization potential that affects the charged body. This image charge phenomenon was explained using the concept of image charge. So, the electron of the attached particle s' image appears through a surface (the surface acts like a mirror), so it is called the image potential. Therefore, the image potential can be generalized to the case of a quantum-dot adsorbed to the graphene. When it approaches the graphene, its energy level will suffer a shift due to the image-shift of the polarized charge on the graphene. We can calculate the image-shift as follows [27]:

$$\Delta E(d) = \frac{e^2}{4d} \tag{1}$$

The above relationship is valid for distances far from the graphene and is not valid for closer distances. Therefore, it was modified to the following formula:

$$\Delta E(d) = \frac{e^2}{4(d+d_o)} \tag{2}$$

,where $d_{\circ}$ represents the location of the image plane, or the screening-length that was used for theoretical treatment as an adjustment parameter. When the adsorbed quantum-dot is in the closest location to graphene, the wave functions of the electrons of the quantum-dot and graphene interfere with each other.

Since the subject of the research is limited to the mechanism of chemical adsorption of quantum-dots, therefore the effect of bonding energy does not play a fundamental role as it would in the chemical adsorption of alkali atoms on the surfaces of transition metals. However, we cannot completely neglect this limit, so it will be considered as a fixed quantity does not depend on distance and spin.

The mathematical model was used in this study is the Anderson-Newns model for chemical adsorption. It is a theory to describe chemical adsorption on the surface. Anderson also described the conditions necessary for the existence of local magnetic states within a single impurity boundary with dissolved states. The Hamiltonian Anderson-Newns model was modified for the case for adsorption of the quantum-dot on the graphene layer as follows:

$$H_A = \sum_G \epsilon_{\vec{G}} c^{\dagger}_{\vec{G}\sigma} c_{\vec{G}\sigma} + E^{\sigma}_{dot} d^{\dagger}_{\sigma} d_{\sigma} + U\left(d^{\dagger}_{\sigma} d_{\sigma}\right)\left(d^{\dagger}_{-\sigma} d_{-\sigma}\right) + \sum_{\vec{G}}\left(V_{\vec{G}\sigma} c^{\dagger}_{\vec{G}\sigma} d_{\sigma} + V^{*}_{\vec{G}\sigma} c_{\vec{G}\sigma} d^{\dagger}_{\sigma}\right) \tag{3}$$

, where $C_{G\sigma}$, $C^{\dagger}_{G\sigma}$ represent the operators of creation and annihilation of the electronic states on graphene and $d_{\sigma}, d^{\dagger}_{\sigma}$ represent the operators of creation and annihilation of the electronic states of the quantum-dot. U represents Coulomb repulsion or Correlation energy. $V_{G\sigma}$ is the strength of interaction and it represents the hybridization term raises from the result of chemisorption on graphene. Upon chemical adsorption, the localized electrons will have a self-energy of localized electrons, which is given by the following relationship:

$$\sum(E,d) = \left|V(d)\right|^2 \int_{-3t}^{3t} \frac{\rho_G\,(E')}{(E-E')+i\lambda} dE' \quad , \quad \lambda \to 0 \tag{4}$$

$\rho_G\,(E')$ represents the density of states for pure graphene. To derive a relationship to calculate the quantum-shift and broadening, we can multiply Eq.(4) by the complex conjugate to complete the mathematical simplification as following:

$$\sum(E,d) = \left|V(d)\right|^2 \int_{-3t}^{3t} \frac{(E-E')\rho_G\,(E')}{(E-E')+\lambda^2}\, dE' - i\left|V(d)\right|^2 \pi \int_{-3t}^{3t} \frac{\rho_G(E')}{\delta(E-E')} dE'$$

$$= \left|V(d)\right|^2 \int_{-3t}^{3t} \frac{(E-E')\rho_G}{(E-E')+\lambda^2}\, dE' - i\left|V(d)\right|^2 \pi\, \rho_G(E') \tag{5}$$

$$Re \sum(E,d) = \wedge(E,d) = \left|V(d)\right|^2 \int \frac{(E-E')\rho_G}{(E-E')+\lambda^2} dE' \tag{6}$$

$$Im \sum(E,d) = \Delta\,(E,d) = -\left|V(d)\right|^2 \pi\, \rho_G\,(E') \tag{7}$$

Where Eq (6) was used to calculate the quantum-shift, while Eq (7) was used to calculate the broadening that results from the chemisorption process on graphene. The density of states for DOS of pure perfect graphene is as following [28]:

$$\rho_G(E) = \begin{cases} 0 & E\langle -3t \\ -\frac{\left(\frac{2}{1+2\ln(3)}\right)t}{E} & -3t\,\langle E\langle -t \\ \frac{2}{[1+2\ln(3)]t^2}|E| & -t\,\langle E\langle t \\ \frac{\left(\frac{2}{1+2\ln(3)}\right)t}{E} & t\,\langle E\langle 3t \\ 0 & E\rangle 3t \end{cases} \tag{8}$$

t represents the hopping term between carbon atoms in the graphene layer. To introduce the effect of distance on both quantum-shift and broadening, we should use the hybridization energy relationship as following [2]:

$$V(d) = V_\circ e^{-\alpha d} \tag{9}$$

, where V$_\circ$ is a constant represents the hybridization energy at graphene $(d = 0)$ and α is an adjustable parameter given by [27]: $\alpha = \sqrt{2\,|\,\varepsilon_d\,|}$, where ε_d represents the energy level of the isolated quantum-dot relative to the Fermi level. In quantum mechanics and quantum statistics, the occupation number that indicates the percentage of quantum levels being filled with particles such as fermions. Therefore, the occupation number will take one of the two values either 0, the level is empty, or equals 1,the level is completely occupied. The concept of occupation number is an expression of the second quantization method, and it also called the second quantization number representation. So, the occupation number at a temperature 0 K is given by:

$$n_{dot}^{\pm\sigma} = \int_{-3t}^{3t} \rho_{dot}^{\pm\sigma}(E,d)dE \tag{10}$$

$\rho_{dot}^{\sigma}\,(E,d)$ represents the density of states of the quantum-dot in the chemisorption, called as local density of states (LDOS) that was introduced by the following:

$$\rho_{dot}^{\sigma}\,(E,d) = \frac{1}{\pi}\,\frac{\Delta(E,d)}{\left(E-E_{dot}^{\sigma}(E,d)-\Lambda(E,d)\right)^2+\Delta^2(E,d)} \tag{11}$$

The quesi-energy level, which gives the local energy level of the quantum-dot in the chemisorption, was defined by:

$$E_{dot}^{\pm\sigma}\,(E,d) = \varepsilon_{dot} + U\,n_{dot}^{\mp\sigma} + \Delta E(d) \tag{12}$$

The surface temperature will take g into our account through the Fermi distribution function $f(E,T)$, hence, the occupation number and the density of states at adsorption will be a function of the distance and temperature at the same time, therefore the occupation number was given by the following expression:

$$n_{dot}^{\pm\sigma} = \int_{-3t}^{3t} \rho_a^{\pm\sigma}\,(E,d)\,f(E,d)dE \tag{13}$$

The Fermi-Dirac distribution function is known as $f\,(E\,,T) = \frac{1}{1+e^{\frac{E-\mu}{k_BT}}}$, where, k_B the Boltzmann constant and $\mu = 0$ for pure graphene.

When an electric field is applied, the ground state energy curves should take a shape similar to that of a single positively charged ion. The ionization of adsorbed atoms can occur when the highest level is occupied by the energy term laying above the Fermi level, which is expressed by |e|Fd [29, 30]. The effect of the electric field strength on the quantum-dot/graphene adsorption system was taken into our calculations by introducing the additional term $\Delta E(F) = |e|Fd_o$ to equation (12) to become in the following form:

$$E_{dot}^{\pm\sigma}(E,d) = \varepsilon_{dot} + Un_{dot}^{\mp\sigma} + \Delta E(d) + \Delta E(F) \tag{14}$$

Therefore, all the other functions will depend on the electric field as well.

III. RESULTS AND DISCUSSION

The image shift energy ΔE(d) was calculated according to Eq.(2). It can be noticed that the image-shift energy decreased at d=0 when the screening length increased. The image-shift energy means that the relationship between the width of the interaction zone and the shift of the energy level of the adsorbed quantum-dot towards the Fermi level is inverse. The values of the constants were chosen in the calculations are:

$$d_\circ = 2.0\ \text{Å} \quad , V_\circ = 1.0\ eV\ , \alpha = 0.01\text{Å}^{-1}\ \ , U = 0.7\ eV\ ,$$
$$\varepsilon_{dot} = -0.5\ eV$$

To demonstrate the response of the quantum-dot/graphene system to the electric field strength, different values were adopted for the strength of the uniform external electric field in both positive and negative directions based on practical research in studying the effect of the electric field for atomic chemisorption on the graphene layer.

A-The effect of positive external electric field on the occupation number and energy levels.

Studying the positive electric field effects on the surface of metals and semiconductors, is considered an important part of scientific research and its applications to a wide range of industries and industrial technologies. These studies and understanding of their significant surface interactions lead to the development of new and useful applications and technologies. The results are explained in the following tables and figures.

TABLE (1): The chemisorption function for the quantum-dot when it adsorbed on graphene(*d*=0) for different values of electric field in positive direction.

ΔE(F) (eV)	$E_{dot}^{\pm\sigma}$ **(eV)**	$n_{dot}^{\pm\sigma}$	d_{ch}**(Å)**
0.01	1.35	0.062	6.4
0.03	1.33	0.061	6.0
0.05	1.31	0.060	5.6
0.07	1.29	0.059	5.3
0.09	1.28	0.058	5.0
0.12	1.25	0.057	4.6
0.15	1.22	0.056	4.3

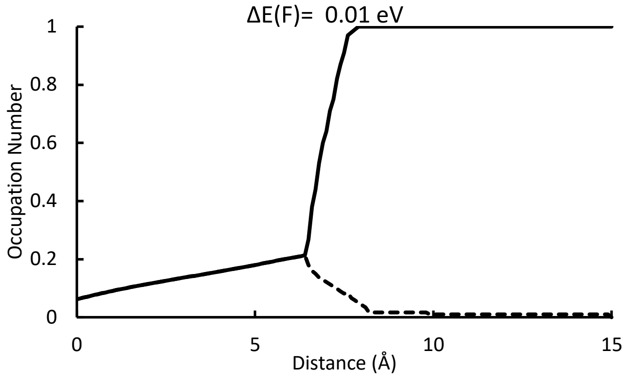

Figure (1-a): The electric field strength (0.005 V/Å) effect on the occupation numbers, the solid line represent $n_{dot}^{+\sigma}$ and the dashed line represent $n_{dot}^{-\sigma}$.

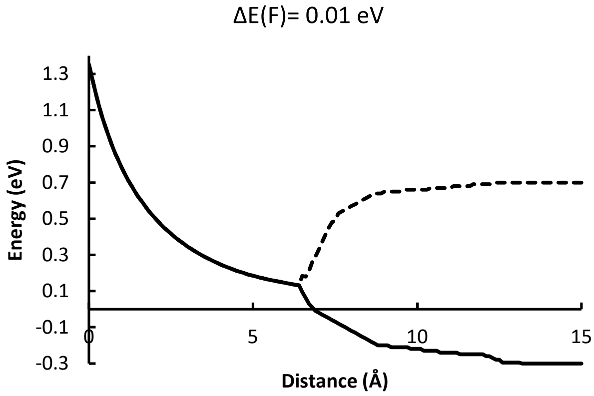

Figure (1-b): The electric field strength (0.005V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

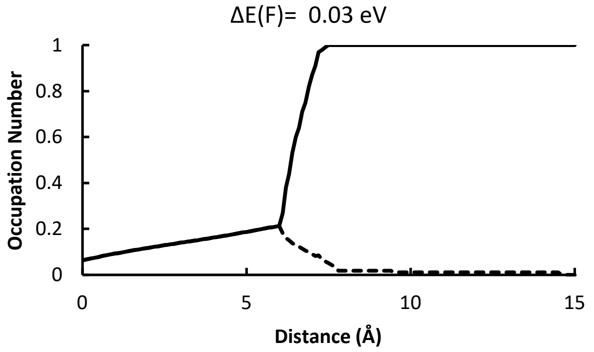

Figure (2-a): The electric field strength (0.015 V/Å) effect on the occupation numbers, the solid line represent $n_{dot}^{+\sigma}$ and the dashed line represent $n_{dot}^{-\sigma}$.

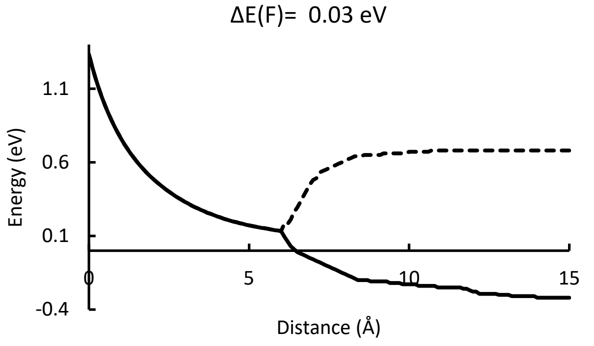

Figure (2-b): The electric field strength (0.015V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

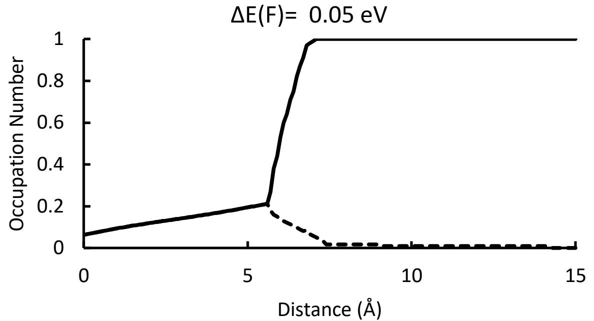

Figure (3-a): The electric field strength (0.025 V/Å) effect on the occupation numbers, the solid line represent $n_{dot}^{+\sigma}$ and the dashed line represent $n_{dot}^{-\sigma}$.

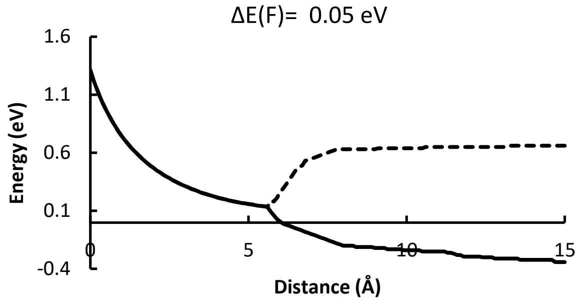

Figure (3-b): The electric field strength (0.025V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

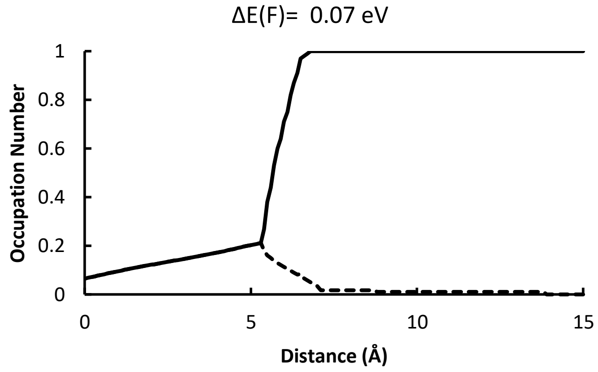

Figure (4-a): The electric field strength (0.035 V/Å) effect on the occupation numbers, the solid line represent $n_{dot}^{+\sigma}$ and the dashed line represent $n_{dot}^{-\sigma}$.

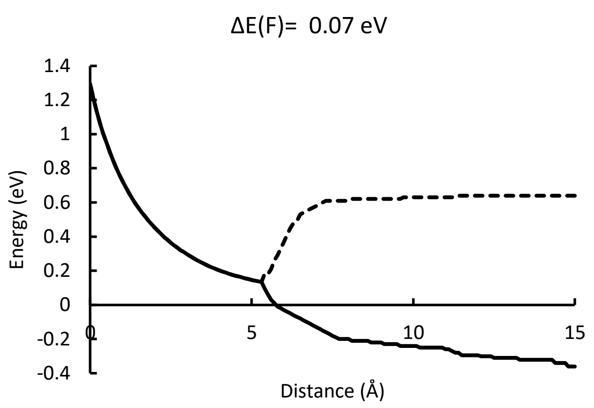

Figure (4-b): The electric field strength (0.035V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

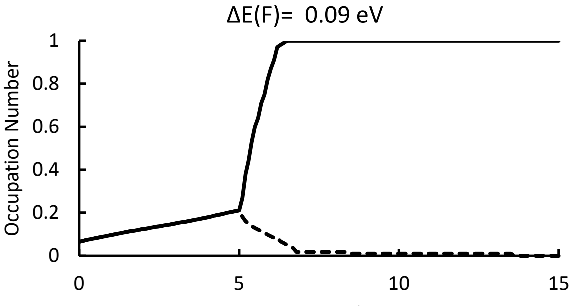

Figure (5-a): The electric field strength (0.045 V/Å) effect on the occupation numbers, the solid line represent $n_{dot}^{+\sigma}$ and the dashed line represent $n_{dot}^{-\sigma}$.

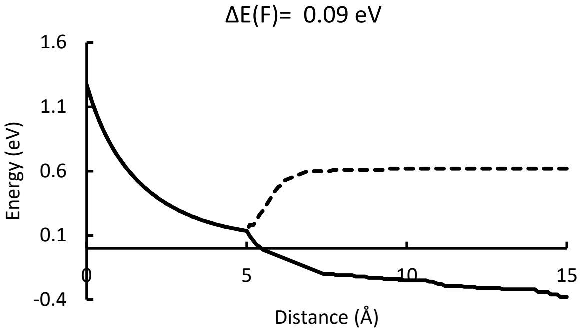

Figure (5-b): The electric field strength (0.045V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

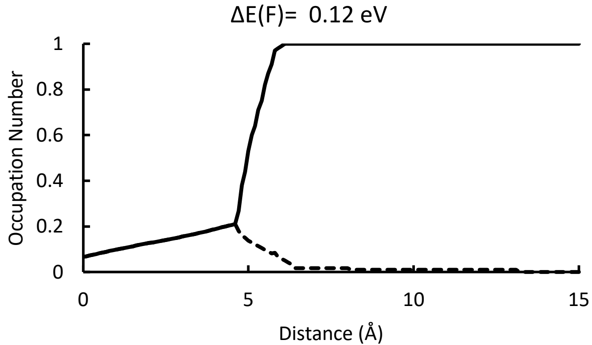

Figure (6-a): The electric field strength (0.06 V/Å) effect on the occupation numbers, the solid line represent $n_{dot}^{+\sigma}$ and the dashed line represent $n_{dot}^{-\sigma}$.

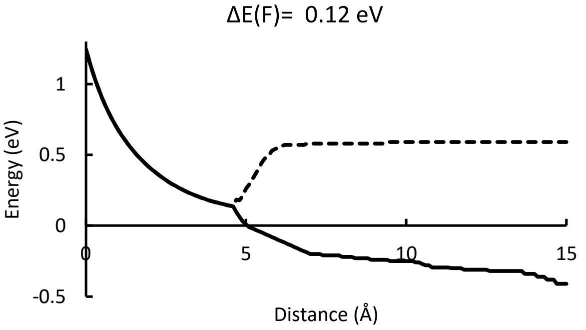

Figure (6-b): The electric field strength (0.06 V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

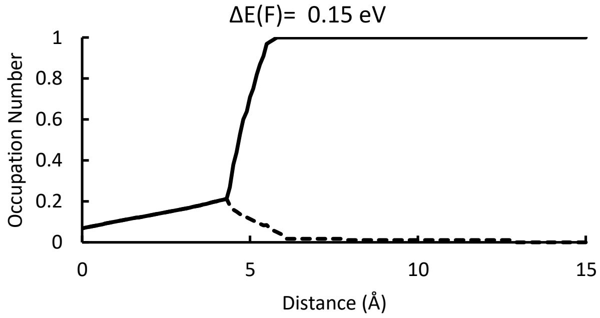

Figure (7-a): The electric field strength (0.075 V/Å) effect on the occupation numbers, the solid line represent $n_{dot}^{+\sigma}$ and the dashed line represent $n_{dot}^{-\sigma}$.

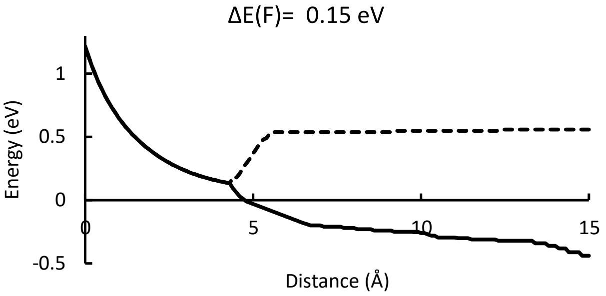

Figure (7-b): The electric field strength (0.075V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

The above results shows that by increasing the external electric field in the positive direction on the graphene layer led to an increase in the energy level and a slight decrease in the occupation number, but this led to a weak adsorption and enhances the possibility of separation of the adsorption quantum-dot. In addition to that, the point of exchange for the magnetic and non-magnetic solutions decreases with increasing field strength, that means the proportionality between F and d_{ch} is inversely proportional.

B- Effect of negative external electric field on the occupation number and energy levels.

This effect can be very important in a variety of applications. By Knowing the effect of a negative electric field can also be used to develop anti-adsorption materials. These materials have the ability to prevent the adsorption of materials on their surfaces. This effect has many applications such as smart surface design and pollution control. Also in the field of manufacturing electronic devices, a negative electric field can affect the chemisorption between different parts of devices. Understanding this effect can help improve the performance of these devices. The results are explained in the following tables and figures.

TABLE(2):The chemisorption function for the quantum-dot when it adsorbed on graphene (*d*=0) for different values of electric field in negative direction.

ΔE(F) (eV)	**$E^{\pm\sigma}_{dot}$ (eV)**	**$n^{\pm\sigma}_{dot}$**	**d_{ch}(Å)**
-0.01	1.35	0.0622	6.4
-0.03	1.33	0.0629	6.0
-0.05	1.31	0.0636	5.6
-0.07	1.29	0.0644	5.3
-0.09	1.28	0.0651	5.0
-0.12	1.25	0.0663	4.6
-0.15	1.22	0.0675	4.3

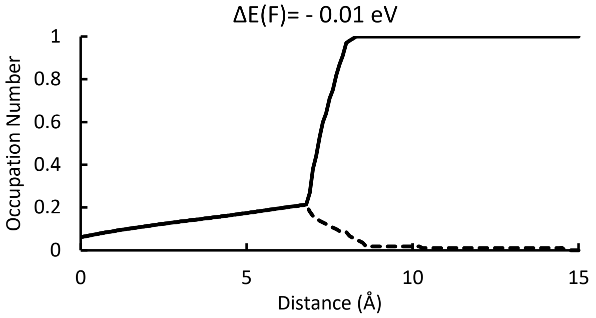

Figure (8-a): The electric field strength (-0.005 V/Å) effect on the occupation numbers, the solid line represent $n^{+\sigma}_{dot}$ and the dashed line represent $n^{-\sigma}_{dot}$.

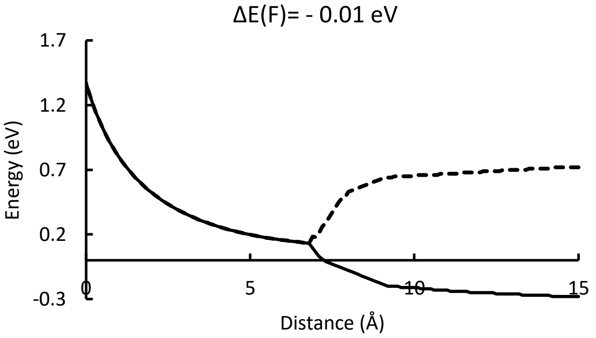

Figure (8-b): The electric field strength (-0.005V/Å) effect on the adsorbed energy levels, the solid line represent $E^{+\sigma}_{dot}$ and the dashed line represent $E^{-\sigma}_{dot}$.

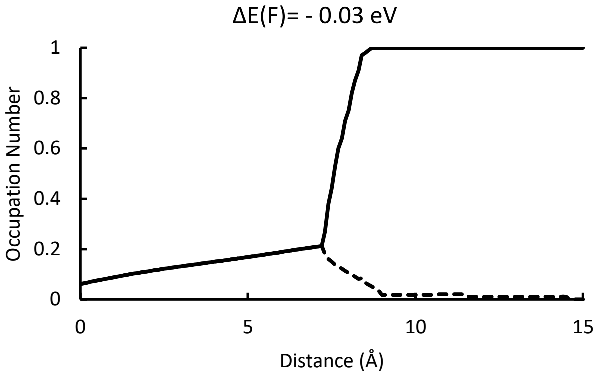

Figure (9-a): The electric field strength (-0.015 V/Å) effect on the occupation numbers, the solid line represent $n^{+\sigma}_{dot}$ and the dashed line represent $n^{-\sigma}_{dot}$.

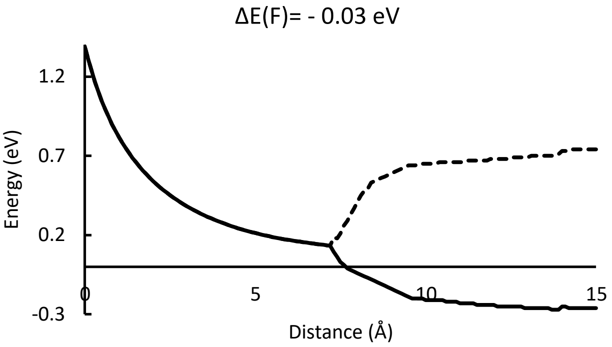

Figure (9-b): The electric field strength (-0.015V/Å) effect on the adsorbed energy levels, the solid line represent $E^{+\sigma}_{dot}$ and the dashed line represent $E^{-\sigma}_{dot}$.

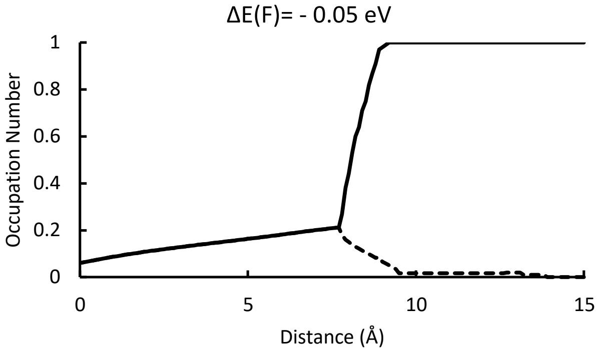

Figure (10-a): The electric field strength (-0.025 V/Å) effect on the occupation numbers, the solid line represent $n^{+\sigma}_{dot}$ and the dashed line represent $n^{-\sigma}_{dot}$.

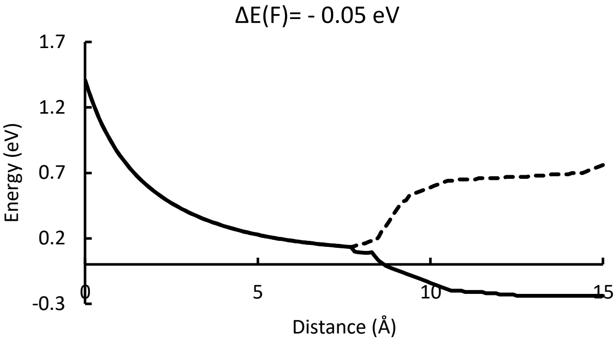

Figure (10-b): The electric field strength (-0.025V/Å) effect on the adsorbed energy levels, the solid line represent $E^{+\sigma}_{dot}$ and the dashed line represent $E^{-\sigma}_{dot}$.

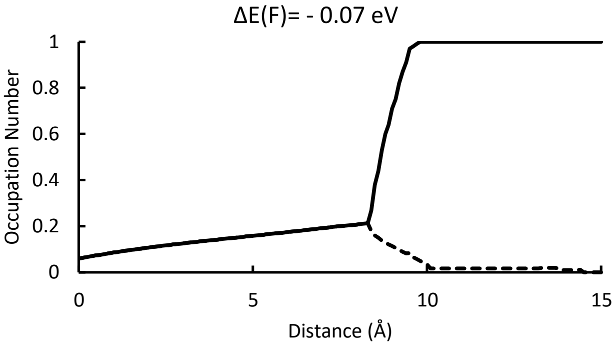

Figure (11-a): The electric field strength (-0.035 V/Å) effect on the occupation numbers, the solid line represent $n^{+\sigma}_{dot}$ and the dashed line represent $n^{-\sigma}_{dot}$.

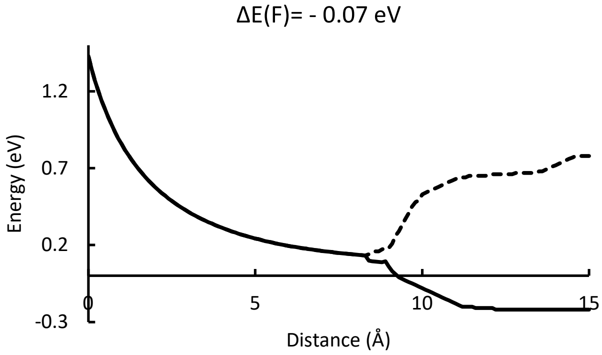

Figure (11-b): The electric field strength (-0.035V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

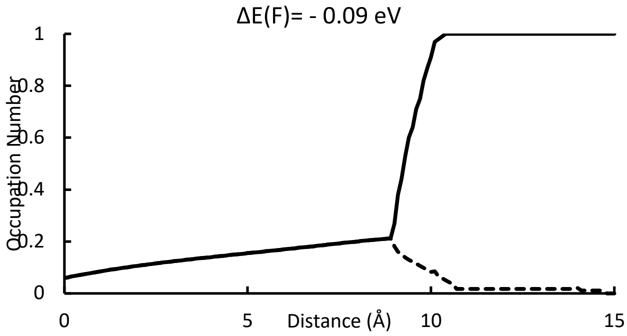

Figure (12-a): The electric field strength (-0.045 V/Å) effect on the occupation numbers, the solid line represent $n_{dot}^{+\sigma}$ and the dashed line represent $n_{dot}^{-\sigma}$.

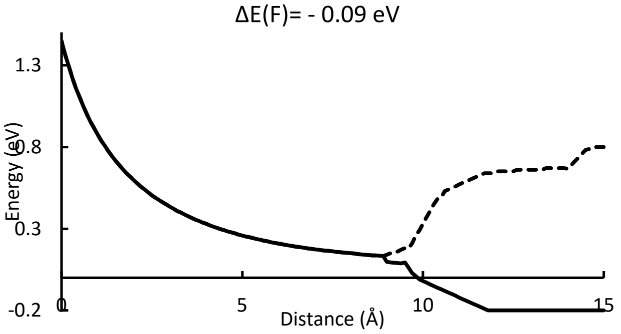

Figure (12-b): The electric field strength (-0.035 V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

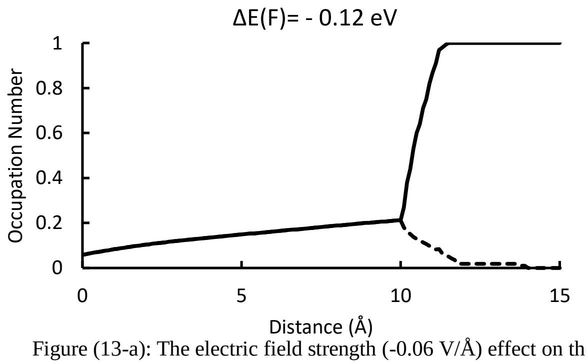

Figure (13-a): The electric field strength (-0.06 V/Å) effect on the occupation numbers, the solid line represent $n_{dot}^{+\sigma}$ and the dashed line represent $n_{dot}^{-\sigma}$.

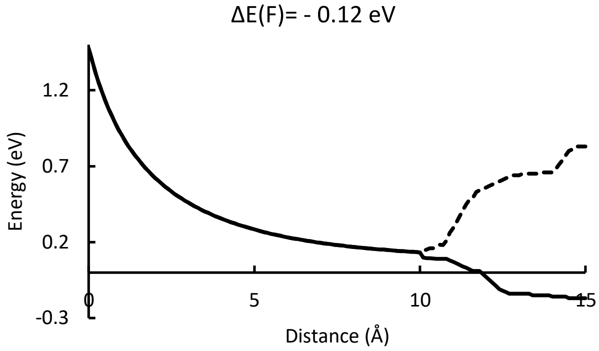

Figure (13-b): The electric field strength (-0.06 V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

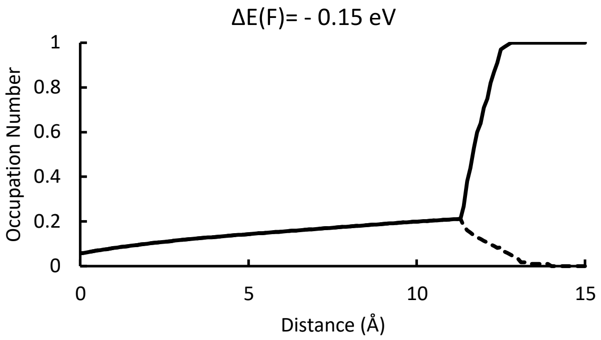

Figure (14-a): The electric field strength (-0.075 V/Å) effect on the occupation numbers, the solid line represent $n_{dot}^{+\sigma}$ and the dashed line represent $n_{dot}^{-\sigma}$.

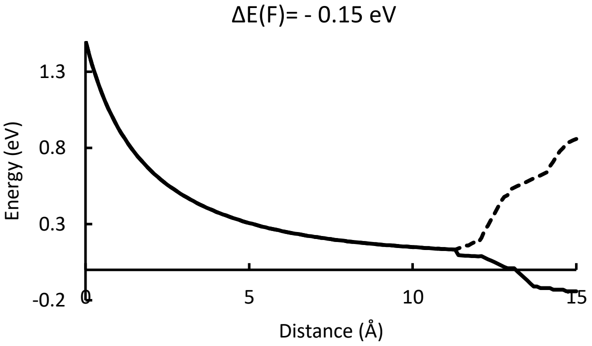

Figure (14-b): The electric field strength (-0.075 V/Å) effect on the adsorbed energy levels, the solid line represent $E_{dot}^{+\sigma}$ and the dashed line represent $E_{dot}^{-\sigma}$.

Our results showed that: by increasing the strength of the external electric field in the negative direction to the graphene layer led to reducing in the energy of the quantum-dot level and increasing the value of the occupation number. This effect enhanced adsorption and increased the difficulty of desorption adsorbed quantum-dot. The point of exchanging the magnetic and non-magnetic solutions decreased with increasing the negative strength of the external electric field, and that means the proportionality here between F and d_{ch} is inversely proportional.

IV. CONCLUSION

The discussed results in our current study are one of the basic and important field of research. The initial conditions for the quantum-dot (initial values of the occupation numbers and the energy levels $E_{dot}^{\pm\sigma}$ ε_{dot}) are $n_{dot}^{+\sigma}=1$,$n_{dot}^{-\sigma}=0$, $E_{dot}^{+\sigma}=\varepsilon_{dot}$. Since, the initial values of quantum-dot functions were at far from graphene. All adsorption functions were calculated so that the chemisorption and the occupation numbers at a certain location d according to the pervious location serve as initial values for it. One of the most important results was determining the type of solution, whether they are magnetic $n_{dot}^{-\sigma}\neq n_{dot}^{+\sigma}$ or non-magnetic $n_{dot}^{-\sigma}=n_{dot}^{+\sigma}$ .By determining the value of the point at which the solutions change of d_{ch} and examining chemisorptuin factors affect the determination of adsorbed energy levels and their occupation numbers. Image-shift effects play an important role in the determining of d_{ch}, then we can determine the length of distance at which chemisorption solutions is non-magnetic and the state of charge as a function of distance.

In addition, the chemisorption functions at d=0 of the quantum-dot, when it adsorbed to the graphene layer, were affected by the application of an external electric field and different values of the field strength in both positive and negative directions $F=|0.005-0.150|\ V/\text{Å}$ The shift of energy level values increased due to the electric field and are also accompanied by a slight increase in the values of the energy levels with a decreasing in the values of the occupation numbers and an decreasing in the values of d_{ch}. Note that the negative electric field influenced more in the chemisorption of the quantum-dot on pure perfect graphene.

CONFLICT OF INTEREST

Authors declare that they have no conflict of interest.

REFERENCES

[1]H. K. Fadel, "Field Desorption of Ions (Atoms) From Solid Surface", M.Sc. Thesis, Dept. of Physics, Univ. of Basrah, Basra, 2002.

[2]H. K. Fadel, A. K. Nokhov and G. M. Mysaev, "The Electric Field Effects on The Chemisorption of Alkalis/Ni systems", *Journal of Dagestan State University*, Vol.6, p.54, 2012.

[3]H. Al-Mahdi, "Electron Transfer Assisted QD-QW-QD Nanostructure System", Ph.D Dissertation, Dept. of Physics, Univ. of Basrah, Basra, 2017.

[4]T. O. Wehling, E. Sasoglu, C. Friedrich, A. Lichtenstein, M. Katsnelson and S. Blugel, "Strength of Effective Coulomb Interactions in Graphene and Graphite", *Phys. Rev. Lett.*, Vol.106, p. 236805, 2011.

[5]Sh. Booyens, L. Gilbert, D. Willock and M. Bowker, "The Adsorption of Ethene on Fe (111) and Surface Carbide Formation". *Catalysis Today*, Vol. 244, p.9137, 2014.

[6]L. E. Brus, "Chemistry and Physics of Semiconductor Nanocrystals", *Ph.D Thesis*, Columbia Universtiy, New York, 2007.

[7]D.J. Norris and M. G. Bawendi, "Measurement and Assignment of the Size-Dependent Optical Spectrum in Cadmium Selenide (CdSe) Quantum-dots", *Phys. Rev. B*, Vol. 53, p.16338, 1996.

[8]J.M. Mukh and F.N. Ajeel, "Manipulation of Atom-Sized Quantum-dot with a Scanning Tunneling Microscope", *Journal of Science - University of Thi Qar*, Vol.4, p.4, 2012.

[9]Michael R. Geller, "Fundamentals of Physics–Vol. II: Quantum Phenomena in Low-Dimensional Systems", eBook: **https://arxiv.org/abs/cond-mat/0106256v1**, 2001.

[10]S. Adam, E. H. Hwang, E. Rossi, and S. Das Sarma, "Theory of charged impurtity scattering in two-dimensional graphene", *Solid State Commun.*, Vol. 149, No.27, p. 1072, 2009.

[11]A. Kuc, T. Heine, and G. Seifert, "Structural and electronic properties of graphene nanoflakes", *Conden. Mat. Phys.*, Vol. 81, No. 8, 2010.

[12]A. H. Mashhadzadeh, A. M. Vahedi, M. Ardjmand, and M. G. Ahangari, "Investigation of heavy metal atoms adsorption onto graphene and graphdiyne surface: A density functional theory study", *Super lattices Microstruc.*, Vol. 100, p. 1094, 2016.

[13]A.K. Geim and K. S. Novoselov, "The rise of graphene", *Nanosci. Tech*, Vol. 6, No.3, p. 11, 2009.

[14]M. Katsnelson, K. Novoselov and A. Geim, "Chiral tunneling and the Klein paradox in graphene", *Nat. Phys.*, Vol. 2, No. 9, p. 620, 2006.

[15] K. Mikhail, "Graphene: carbon is one of the most intriguing element in the Periodic Table", *Materials today*, Vol. 10, No. 1, p. 20, 2007.

[16]Md Sohanur, B. Mondal et.al., 'Overview of Graphene as Promising Electrode Materials for Li-ion Battery', *International J.Sci.Res. and Engin.Deve.***,** Vol. 4, Issue 6, 2021.

[17]K. S. Novoselov, Z. Jiang, Y. Zhang, SV. Morozov , "Room-Temperature Quantum Hall Effect In Graphene", *Science*, Vol. 315, p. 150, 2007.

[18]T. Ohta, A. Bostwick et.al., "Controlling the electronic structure of bilayer graphene", *Science*, Vol. 313, No. 5789, p. 951, 2006.

[19]Y. Zhang, Y. W. Tan, H. L. Stormer and P. Kim, "Experimental observation of the quantum Hall effect and Berrys phase in graphene", *Nature*, Vol. 438, No. 7065, p. 201, *2005*.

[20]K. S. Novoselov, A.K. Geim et.al., "Two-dimensional gas of massless Dirac fermions in graphene", *Nature*, Vol. 438, No. 7065, p. 197, 2005.

[21]A. Jang, S. Adam et.al., "Tuning the effective fine structure constant in graphene: Opposing effects of dielectric screening on short-and – long –range potential scattering", *Phys. Rev. Lett.*, Vol. 101, No. 14, p.1, 2008.

[22]J. Martin Akerman, G. Ulbricht et.al, "Observation of electron-hole puddles in graphene using a scanning single-electron transistor", *Nat.Phys.*, Vol. 4, No. 2, p. 144, 2008.

[23]M. Ishigami, J. Chen et.al., "Atomic structure of graphene on SiO_2", *Nano Lett.*, Vol. 7, No. 6, p. 1643, 2007.

[24]G. Li and E. Y. Andrei, "Observation of Landau levels of Dirac fermions in graphite", *Nat. Phys.*, Vol. 3, No. 9, p. 623, 2007.

[25]D. Sharpiro, J. Eigner and G. Greenberg, "Inability of Thymine-Dependent Mutants of Bacteriophage T4 to Induce", *Proc.Nat.Aca.Sci.*, United States, Vol. 53, No. 22, p. 874, 1965.

[26]X. Song, Q. Chen et.al., "Effect of Chlorine Adatoms on Small Lithium Nanocluster Adsorbed Graphene", *Chem. Phys. Lett.*, Vol. 738, p. 136896, 2020.

[27]K. Nakada and A. Ishii, "DFT Calculation for Adatoms Adsorption on Graphene", *Graphene Simulation.*, 2011.

[28]S. Yu. Davydov, "Small atomic clusters on metal, semiconductor, and graphene: A model approach", *Phys.Sol. State*, Vol.54, No.8, p.2329, 2012.

[29]C. Kim, B. Kim, S. Lee, C. Jo and Y. Lee, "Effect of Electric Field on the Electronic Structure of Carbon Nanotubes", *Appl. Phys. Lett.*, Vol. 79, p. 1187, 2001.

[30]Y. Guo, W. Guo, C. Chen, "Tuning Field-induced Energy Gap of Bilayer Graphene via Interlayer Spacing", *Appl. Phys. Lett.*,Vol.92, p.243101, 2008.