

Theoretical Study in the Chemisorption of Alkali Atoms on the Graphene Sheet*

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Abstract

We use Newns-Anderson model to study the chemisorption of alkali atoms (Na and K) on perfect graphene. The self-consistent solutions for alkali atoms occupation levels show that the physical solution (for K atom) is nonmagnetic for all normal distance values from the graphene sheet, while for Na atom, it is nonmagnetic at small distance and magnetic for relatively large distance . Accordingly, the type of magnetization determines the dominant part of the chemisorption energy on the adatom. The ionic part of the chemisorption energy is the dominant one at graphene sheet, which gives the obvious description to the type of alkali bonding formed with the graphene.

Key words: Graphene, Chemisorption, magnetization, Nanotechnology.

• It is a part of Ph.D. thesis submitted by the first author.

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1: Introduction

Graphene are made out of carbon atoms arranged in hexagonal structure. The structure can be seen as a triangular lattice with a basis of two atoms per unit cell ⁽¹⁾.

As graphene has an unusual band structure that leads to interesting effects and potentially to useful electronic devices ⁽²⁾. It becomes an excellent candidate for the next generation of electronic materials due to its amazing electronic and transport properties. An ideal graphene is semi-metallic and nonmagnetic ⁽³⁾.

The adsorption of atoms or molecules on solid may undergo phase transitions. The adsorption process may involve the motion of the adsorbed atom or molecule coupled to all the degrees of freedom of solid surface. Most of the problems involved have counterparts in surface physics or molecular physics or chemistry, but the presence of adatoms or molecules on solid surface increases the complexity of them, both from experimental and a theoretical point of view ⁽⁴⁾.

The rapid experimental development of nano science provides us with more observation on chemisorption of species on solid.

Theoretically, two different approaches are taken into consideration. **The first one** is to include everything in the electronic structure calculations of the electronic structure. Most of these are in the sense that they do not require any input about the system under study except the charges and geometrical arrangement of the constituent atoms. All of the calculations make approximations in their treatment of the electron – electron interactions ⁽⁵⁾. **The second** is to devise simple models that can capture only the essential physics. This approach is very well suited to bring out the important concepts and physical pictures.

In our study, we shall use one of the second type models to study the time – independent chemisorption process on graphene incorporating the spin on the adsorbed atom, this model is Newns – Anderson model ^(6,7).

Our model calculation takes the following (adatom/graphene) system physical features into consideration,

1. All the parameters that concerned to the type of atom which adsorbed on graphene sheet, i.e. the ionization energy of the atom, the correlation energy on the adsorbed atom and the position of the image plane.
2. The system electronic structure and then the quantum coupling effects which are expressed by the broadening chemisorption function and the quantum shift. Both are related to the strength of interaction between the adsorbed atom and the graphene sheet.

Our study comprises three main lines of investigation. The first is the calculation of the broadening and the quantum shift as a function of energy and the normal distance between the atom and the graphene sheet, then accordingly the adsorbate density of states on the graphene sheet. The second is the calculation of the net charge and the magnetization on the adsorbed atom. While the third is to calculate the ionic and the metallic parts of the chemisorption energy.

The Chemisorption of species on solid surface can be defined as the bonding of atoms or molecules to a solid surface and refers to bonds of chemical strength, as opposed to physisorption which refers to weaker bonds that can only be stabilized on the surface at low temperatures. Because chemisorption involves energies that are sizable on chemical scale the chemisorption process is often associated with the breaking of bonds. The description of the chemisorption bond on solid requires a detailed understanding of the electronic structure of atoms and molecules outside solid surface. The determination of the geometrical structure of solid surface with chemisorbed species is developing into an enormous industry related to surface crystallography.

The adsorption of atoms or molecules on solid may undergo phase transitions. The adsorption process may involve the motion of the adsorbed atom or molecule coupled to all the degrees of freedom of solid surface. Most of the problems involved have counterparts in surface physics or molecular physics or chemistry, but the presence of adatoms or molecules on solid surface increases the complexity of them, both from experimental and a theoretical point of view ⁽⁴⁾.

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2. The Theoretical Treatment

In the second quantization form, the model Hamiltonian of the combined system is ^(6,7,8),

$$H = \sum_{k\sigma} E_k^\sigma n_k^\sigma + \sum_{\sigma} E_a^\sigma n_a^\sigma + U n_a^\sigma n_a^{-\sigma} + \sum_{k\sigma} (V_{ak}^\sigma C_a^{\sigma+} C_k^\sigma + V_{ka}^\sigma C_k^{\sigma+} C_a^\sigma) \quad \dots(1)$$

Where, E_k^σ and n_k^σ are the energy levels with set of quantum numbers k and the corresponding occupation numbers in the surface energy band respectively for spin σ . E_a^σ is the spin dependent effective energy level of the adsorbed atom and n_a^σ is the corresponding occupation number.

It is well known that there is a difference in energy between the atom's ionization V_i and the affinity V_A energy levels (far away from a surface) due to electron-electron interaction. This difference is given by ⁽⁵⁾,

$$U = V_i - V_A \quad \dots\dots (2)$$

As the atom approaches to a surface, the ionization and affinity energy levels are shifted towards each other, which means that the value of U (*i.e.* its effective value, which will be denoted as U_{eff}) decreases as the atom moves towards the surface due to the electron-electron correlation interaction⁽⁹⁾. The treatment of U_{eff} problem, *i.e.* its formulation and its dependence on distance from surface Z , is one of the difficulties that faced by researchers. The Coulombic correlation energy U on the atom may be assumed for simplicity to be infinite, zero or as a constant ($= V_i - V_A$), in spite of taking it into considering provide high accuracy in describing the charge exchange processes between the atom and the surface in particular at the closest approach.

And as our study is concerned to the chemisorption of atom on graphene sheet, the intra-atomic correlation interaction will be taken into consideration in our model calculation.

The correlation energy can be calculated, as a function of the vertical distance (Z) between the adatom and the surface, by using the following relation⁽¹⁰⁾,

$$U_{\text{eff}}(Z) = V_i - V_A - 2\Delta E(Z) \quad \dots (3)$$

With, $\Delta E(Z)$ is the image shift which takes the image effect into consideration. U_{eff} is Z -dependent through out the image shift $\Delta E(Z)$.

The image interaction between the electrons in the adatom and the surface (at certain separation, *i.e.* normal distance which represents by Z) is given by⁽¹¹⁾,

$$\Delta E(Z) = e^2 / [4(Z + Z_0)] \quad \dots (4)$$

Then by taking image effect and the correlation effect, the atomic energy level E_a^σ ($E_a^{-\sigma}$) with spin up (spin down) is written as^(12,13),

$$E_a^{\pm\sigma}(Z) = E_a^0 + \Delta E(Z) + U_{\text{eff}} n_a^{\mp\sigma} \quad \dots (5)$$

E_a^0 is equal to $(\phi_0 - V_i)$, ϕ_0 is the surface work function, n_a^σ is the occupation number of the atomic energy level of spin up (*i.e.* E_a^σ),

$$n_a^\sigma = \int_{u_\sigma}^{\phi_\sigma} f(E, T) \rho_{ad}^\sigma(E) dE \quad \dots (6)$$

With u_σ is the energy of the band bottom. ρ_{ad}^σ is the local density of states on the adatom (which will be highlighted extendedly) and $f(E, T)$ is the Fermi distribution function for the graphene sheet,

$$f(E, T) = 1 / (1 + e^{(E/k_B T)}) \quad \dots (7)$$

k_B is the Boltzmann constant and T is the temperature.

The local density of states associated with each atomic level of spin σ ($-\sigma$) is a Lorentzian distribution centered at E_a^σ ($E_a^{-\sigma}$) as,

$$\rho_{ad}^\sigma(E) = \frac{1}{\pi} \frac{\Delta^\sigma(E)}{[E - E_a^\sigma - \Lambda^\sigma(E)]^2 + [\Delta^\sigma(E)]^2} \quad \dots(8)$$

Where E_a^σ is the effective energy level of the adsorbate atom with spin σ . $\Delta^\sigma(E)$ and $\Lambda^\sigma(E)$ are the energy dependent chemisorption functions (the adatom energy level broadening and the quantum shift due to coupling interaction between the adsorbate atom and the surface respectively),

$$\Delta^\sigma(E) = \pi \sum_k |V_{ak}^\sigma|^2 \delta(E - E_k) \quad \dots (9)$$

where⁽¹⁴⁾, $V_{ak}^\sigma = v_k V_0^\sigma$ and,

$$\rho_G(E) = \sum_k |v_k|^2 \delta(E - E_k) \quad \dots\dots (10)$$

$\rho_G(E)$ is the graphene sheet density of states.

Then equation (9) can be rewritten as,

$$\Delta^\sigma(E) = \pi |V_0^\sigma|^2 \rho_G(E) \quad \dots\dots(11)$$

V_0^σ is the strength of interaction between the adatom and the graphene sheet. The quantum shift can be rewritten as,

$$\Lambda^\sigma(E) = \frac{1}{\pi} P \int d\hat{E} \frac{\Delta^\sigma(\hat{E})}{E - \hat{E}} \quad \dots\dots(12)$$

We get use of the density of states for the perfect graphene⁽¹⁵⁾ (see fig.(1)) to study and investigate the chemisorption process of atoms on graphene sheet. According to the best fitting, we get the following formula,

$$\rho_G(E) = \sum_{n=1}^{13} [a_n + b_n (E - E_{p_n})^2] \quad \dots (13)$$

n refers to the best fitted regions. The best fitted graphene density of states is presented in Fig. (2), with ,

$$b_n = C_n / (E_{f_n} - E_{p_n})^2 \quad \dots\dots (14)$$

The coefficients $a_n, C_n, E_{p_n}, E_{f_n}$ are all presented in Table. (1).

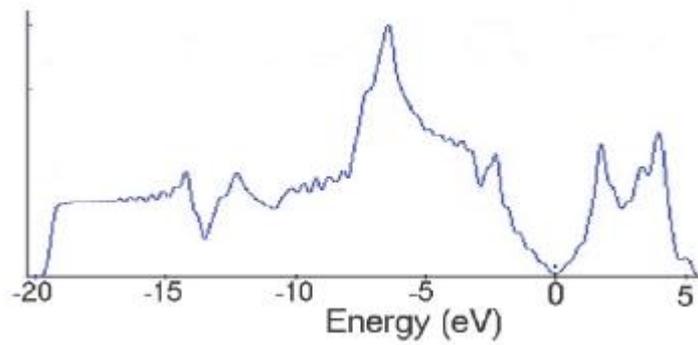


Fig.(1): The DFT graphene density of states⁽¹⁵⁾

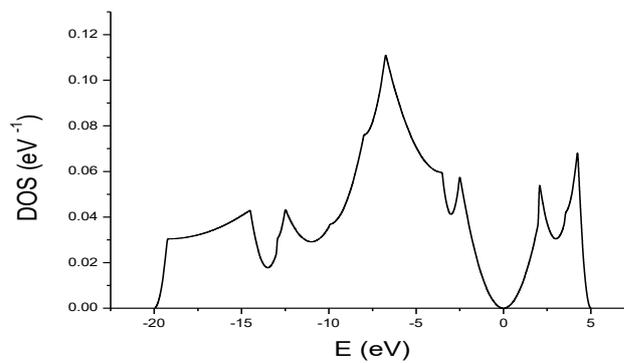


Fig.(2): The fitted graphene density of states

Table (1) : The fitting parameters for graphene density of states shown in Fig.(2)

n	$a_n (\frac{1}{eV})$	$E_{i_n} (eV)$	$E_{p_n} (eV)$	$E_{f_n} (eV)$	$c_n (\frac{1}{eV})$
1	0.0	-20.0	-20.0	-19.25	0.24
2	0.24	-19.25	-19.25	-14.5	0.1
3	0.14	-14.5	-13.5	-13.0	0.2
4	0.24	-13.0	-13.0	-12.5	0.105
5	0.23	-12.5	-11.0	-10.0	0.115
6	0.29	-10.0	-10.0	-8.0	0.31
7	0.6	-8.0	-8.0	-6.75	0.28
8	0.47	-8.0	-3.5	-3.5	0.41
9	0.325	-3.5	-3.0	-2.5	0.135
10	0.0	-2.5	0.0	2.0	0.46
11	0.24	2.0	3.0	3.5	0.22
12	0.33	3.5	3.5	4.25	0.22
13	0.0	4.25	5.0	5.0	0.55

The self-energy due to coupling interaction between (perfect) graphene sheet and an adatom can be written as⁽¹⁶⁾,

$$\sum \sigma(E) = |V_0^\sigma|^2 P \int \frac{\rho_G(E')}{E - E'} dE' \quad \dots\dots (15)$$

By substituting eq.(13) in eq.(15) one can solve the integration analytically to get,

$$\sum \sigma(E) = i \Delta^\sigma(E) + \Lambda^\sigma(E) \quad \dots\dots (16)$$

$\Delta^\sigma(E)$ and $\Lambda^\sigma(E)$ represent the chemisorption functions , i.e. the adatom energy level broadening and its quantum shift (due to coupling interaction) respectively.

Now, we write,

$$\Delta^\sigma(E) = \pi |V_0^\sigma|^2 \sum_{n=1}^{13} [a_n + b_n (E - E_{p_n})^2] \dots (17)$$

and ,

$$\Lambda^\sigma(E) = |V_0^\sigma|^2 \sum_{n=1}^{13} \int_{E_{i_n}}^{E_{f_n}} \frac{(a_n + b_n E_{p_n}) - 2b_n E_{p_n} E' + b_n E'^2}{E - E'} dE' \quad \dots (18)$$

Which is solved analytically to get ,

$$\Lambda^\sigma(E) = |V_0^\sigma|^2 \sum_{n=1}^{13} \left([b_n (2E_{p_n} - E)E - (a_n + b_n E_{p_n}^2)] \ln \left(\frac{E - E_{f_n}}{E - E_{i_n}} \right) - 2b_n (E - E_{p_n})(E_{f_n} - E_{i_n}) - \frac{b_n}{2} (E_{p_n}^2 - E_{i_n}^2) \right) \quad \dots (19)$$

3.The Chemisorption Energy

The chemisorption energy can be defined as the change in the ground state energy on switching on the coupling between the graphene sheet and the adatom. It is well-known that the bond formed between the adatom and the metal surface can be divided into an ionic part and metallic part. This bond energy might be called a delocalization energy, results from allowing the valence electron of the adatom to spread throughout the graphene and the graphene electrons to spread into the region of the atom. In this way the kinetic energies of all electrons are reduced by relaxing slightly the geometric confinement of both the graphene sheet and atomic electrons. The bond formed between the atom and the graphene sheet can be divided into metallic part and ionic part.

The expression for the metallic chemisorption energy is given by ⁽¹²⁾,

$$E_m(Z) = \sum_{\sigma u_0} \int_{\phi} E f(E, T) \rho_{ad}^\sigma(E) dE - U_{eff} n_a^\sigma n_a^{-\sigma} \dots (20)$$

The initial state (at $Z = \infty$) is an atom and a graphene sheet separated by "infinite" distance,

$$E_m(\infty) = \sum_{\sigma u_0} \int_{\phi} E f(E, T) \delta(E - E_a^0) dE \quad \dots (21)$$

$$E_m(\infty) = E_a^0 f(E_a^0, T) \\ = (\phi - V_i) \Theta(V_i - \phi) \quad \dots (22)$$

With Θ is unit step function.

$$\Theta(X) = \begin{cases} 1 & X \geq 0 \\ 0 & X < 0 \end{cases} \quad \dots (23)$$

While the final state is an interacting adatom and graphene sheet separated by an equilibrium distance Z .

As the atom is brought to the graphene sheet, the sharp state broadens and overlaps with the graphene band energy levels such that the effective charge number of the atom is a function of distance and temperature⁽¹⁰⁾,

$$Z_{eff}(Z) = 1 - n_a^\sigma(Z) - n_a^{-\sigma}(Z) \quad \dots (24)$$

The attractive force between the effective charge $eZ_{eff}(Z)$ and its image is $-\frac{e^2 Z_{eff}^2(Z)}{4(Z + Z_o)^2}$ with Z_o is an adjustable parameter which determines the position of the image plane. The work to bring the effective charge from $Z' = \infty$ to $Z' = Z$ is

$$W(Z) = -e^2 \int_Z^\infty \frac{Z_{eff}^2(Z')}{4(Z + Z_o)^2} dZ' \quad \dots (25)$$

This integration must be solved numerically.

Now, the chemisorption energy can be calculated by using the following relation,

$$E_{ch}(Z) = E_m(Z) + W(Z) \quad \dots (26)$$

and the bonding energy,

$$E_{bond} = E_{ch}(Z_o) - E_{ch}(\infty) \quad \dots (27)$$

Since, $W(\infty) = 0$ and $E_m(\infty)$ is given by eq. (22), then,

$$E_{bond} = E_{ch}(Z_o) - (\phi - V_i) \Theta(V_i - \phi) \quad \dots (28)$$

4. The Calculations and the Results

In order to achieve all these calculations, eq. (5) and (6) are solved self-consistently. The work function is given by the energy difference between the Fermi level E_F and the vacuum level. The work function of graphene sheet used in our calculation can be approximately given by 5.0 eV⁽¹⁵⁾. The electronic levels are filled using Fermi-Dirac statistics with a value of temperature $T=300K$. All the parameters that used in our calculations are presented in table (2).

Table (2): The adatom/graphene system parameters.

Atom	V_i (eV)	$\emptyset-V_i$ (eV)	V_A (eV)	R_i (A°)	V_0 (eV)	Z_0 (A°)
Na	5.14	-0.14	0.55	0.97	0.5	3.6
K	4.34	0.66	0.50	1.33	0.5	4.5

Since R_i represents the atom radius and Z_0 is the closest approach and V_0 is the strength of hybridization. The values of V_0 and Z_0 are considered as adjustable parameters.

Our model calculation is used to investigate and study the chemisorption of alkali atoms (Na and K) on the graphene sheet. The alkali adatom/graphene system is also modeled by having an alkali atom on graphene sheet. The charge on the alkali adatom will be analyzed to evaluate the amount of electron transfer between the alkali adatom and the graphene layer. The calculation of the chemisorption energy is the most important because it provides useful information for a better understanding of the growth behavior of metal nanostructures formation on graphene.

The hybridization function and the quantum shift are presented in fig. (3) and fig. (4) respectively as a function of the energy system at $Z=Z_0$ for the alkali atoms used in our study. The values of Z_0 used in our calculations are presented in table (1), these values are not chosen arbitrary. The over mentioned note is also right to the values of the coupling interaction strength which are also presented in table (1), both are considered to be adjustable parameters. Accordingly, at $Z=Z_0$, the adsorbate density of states for each atom will be spin independent, i.e. $\rho_{ad}^\sigma(E) = \rho_{ad}^{-\sigma}(E)$, see fig.(5). In fig. (5), the energy peaks are shifted towards the positive higher energy as the ionization energy decreases.

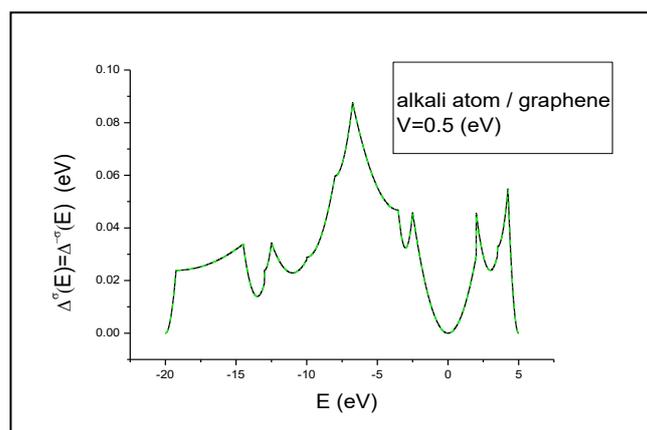


Fig. (3): The broadening function as a function of E for the systems alkali atom/graphene calculated at $Z=Z_0$.

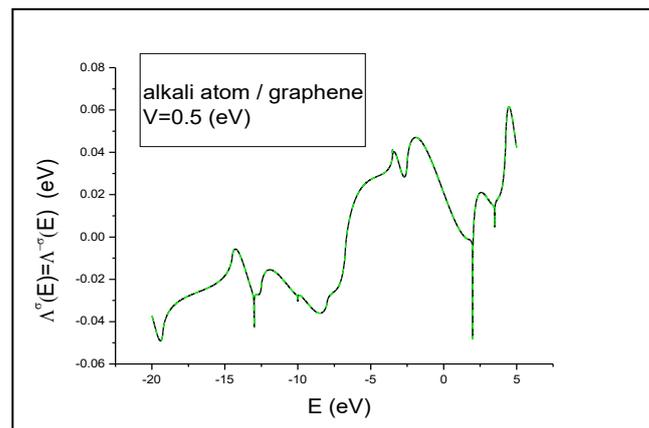


Fig. (4): The quantum shift as a function of E for the systems alkali atom/graphene calculated at $Z=Z_0$.

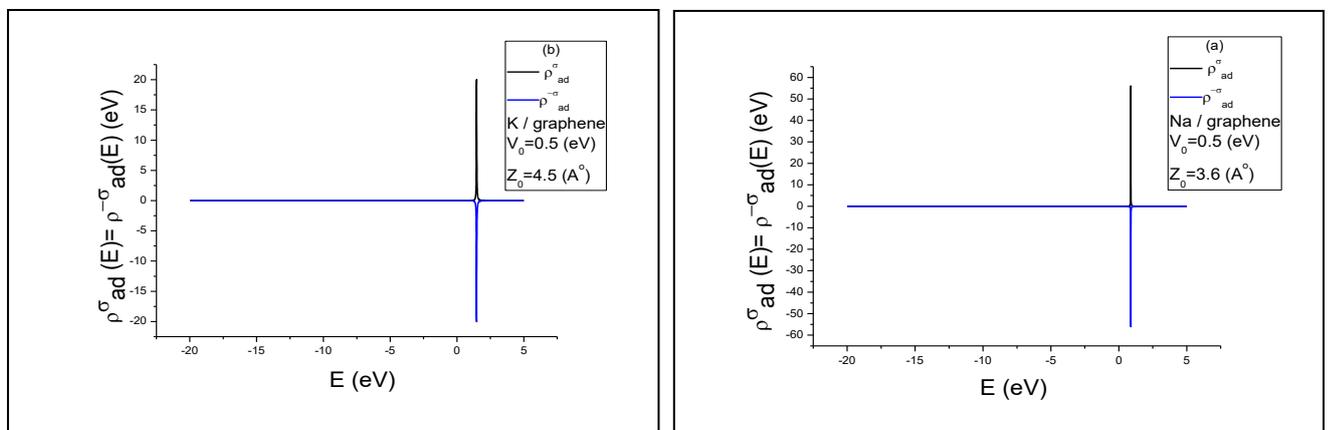


Fig. (5): The adsorbate density of states calculated at $Z=Z_0$ for the alkali atom/graphene systems

Fig. (6) shows the occupation numbers $n_a^{\pm\sigma}$ as a function of distance. The self-consistent solution for Na atom at relatively large distance is magnetic, then at certain distance ($Z=Z_{ch}$) the solution is changed to nonmagnetic one. While for the other alkali atom K, the solution is nonmagnetic for all distances. The values of Z_{ch} for Na atom is 14.3001\AA^0 . The values of Z_{ch} for Na atom can be controlled experimentally by several effects such as the effect of magnetic field on the atom. The corresponding energy levels $E_a^{\pm\sigma}$ are shown in fig. (7), where $E_a^{\sigma} = E_a^{-\sigma}$ for the nonmagnetic state. As the state is nonmagnetic, i.e. there is no net spin on the adsorbed atom, the magnetization is zero (see fig. (8)). For Na, as the atom moves towards the graphene sheet, i.e. for $(0 \leq Z_0 \leq Z_{ch})$, the local magnetic moment is non-vanishing. Since the condition to form a magnetic moment on the atom is determined by calculating the spin-dependent occupation numbers. It is evident from eq.(6) that the determination of the spin-dependent occupation numbers requires the self-consistent calculation for the adsorbate density of states, which incorporates the broadening of the atom energy level due to the hybridization with the sea of Dirac electrons in graphene. A localized moment is

formed at the adatom whenever there is an imbalance in the spin dependent occupation numbers at the level.

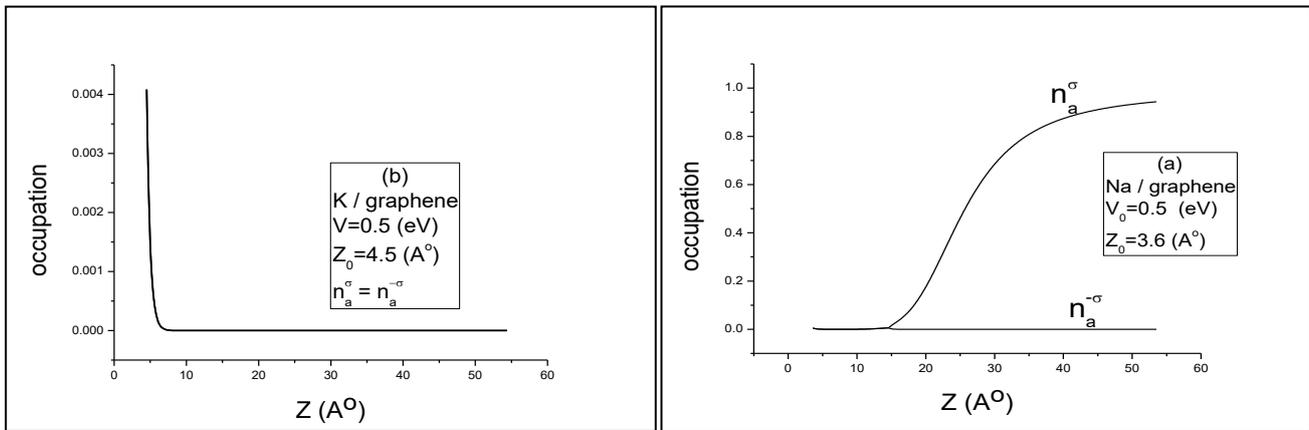


Fig. (6): The occupation numbers on the alkali adatoms as a function of distance

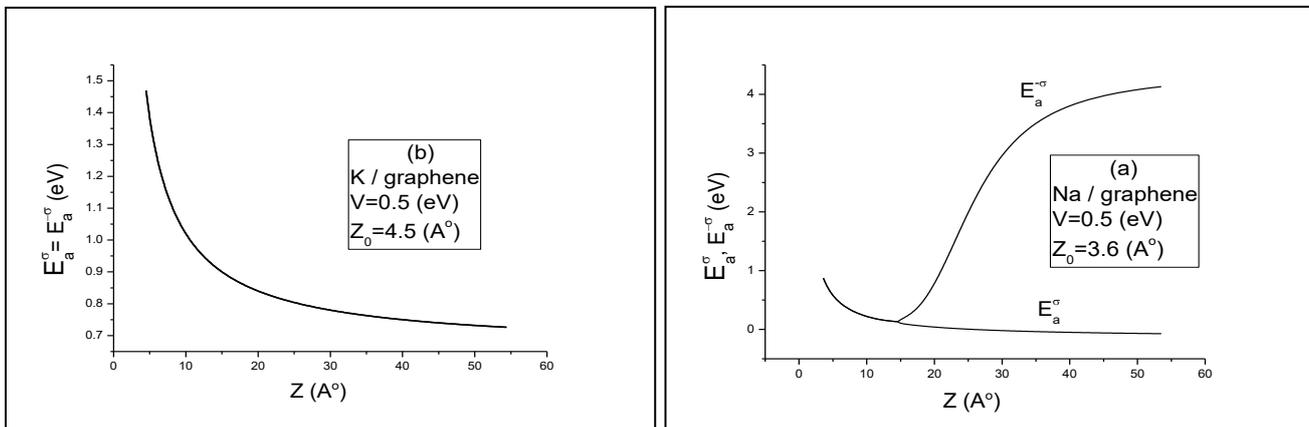


Fig. (7): The alkali adatoms energy levels as a function of distance.

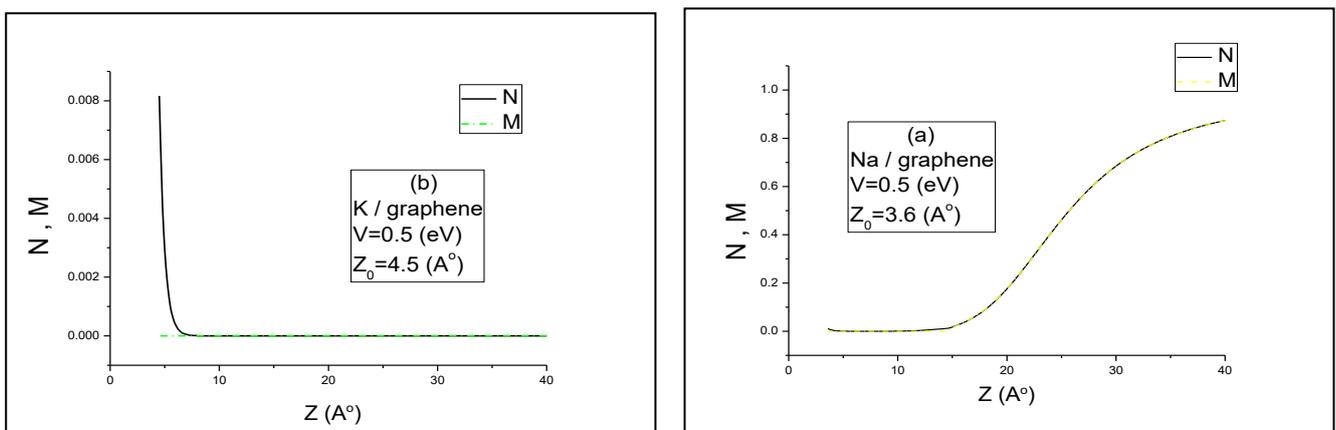


Fig. (8): The total charge and the magnetization on the alkali adatoms as a function of distance.

The effective charge on the adatoms is shown in fig. (9). The value of $Z_{\text{eff}} = 1$ means that $n_a^\sigma = n_a^{-\sigma} = 0$ (the solution is nonmagnetic) and the value of $Z_{\text{eff}} = 0$ means $n_a^\sigma = 1, n_a^{-\sigma} = 0$ (the solution is magnetic).

The portions of the chemisorption energy for the alkali/graphene systems are also presented in fig.(10). The ground state energy of the system Na/graphene is metallic for $Z > 14.3001\text{\AA}^\circ$ and it is ionic for $Z < 14.3001\text{\AA}^\circ$, where $(\emptyset - V_i)$ value is negative for the Na atom. Which means that the atom energy levels of Na atom at relatively large distance, are lying below Fermi energy. For K atom, the ground state energies are ionic where $(\emptyset - V_i)$ are positive. Our calculations show that the alkali adatoms chemisorption on graphene release their valance electron easily and act as good agents for n-doping of graphene. Therefore the interaction between alkali adatoms and graphene is mainly ionic (see table (3)). The total chemisorption energies are shown in fig. (11).

The values of the metallic and ionic chemisorption energies at $Z=Z_0$ are presented in table (2) where the ionic portion is larger than the metallic portion for all alkali atoms. One can get use of the adjustable parameters V_0 and Z_0 to find the experimental data of the chemisorption energy.

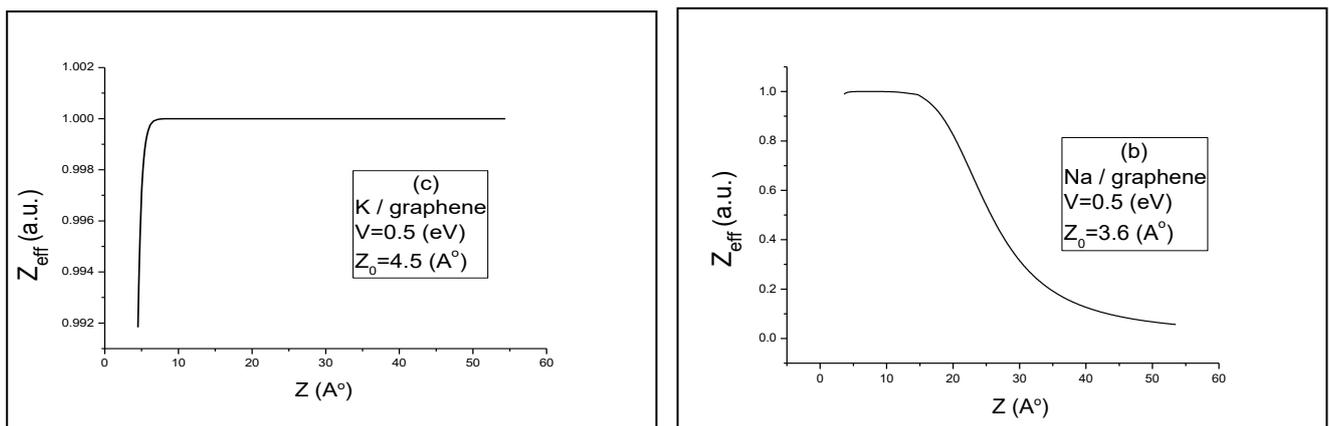


Fig. (9): The effective charge on the alkali adatoms as a function of distance.

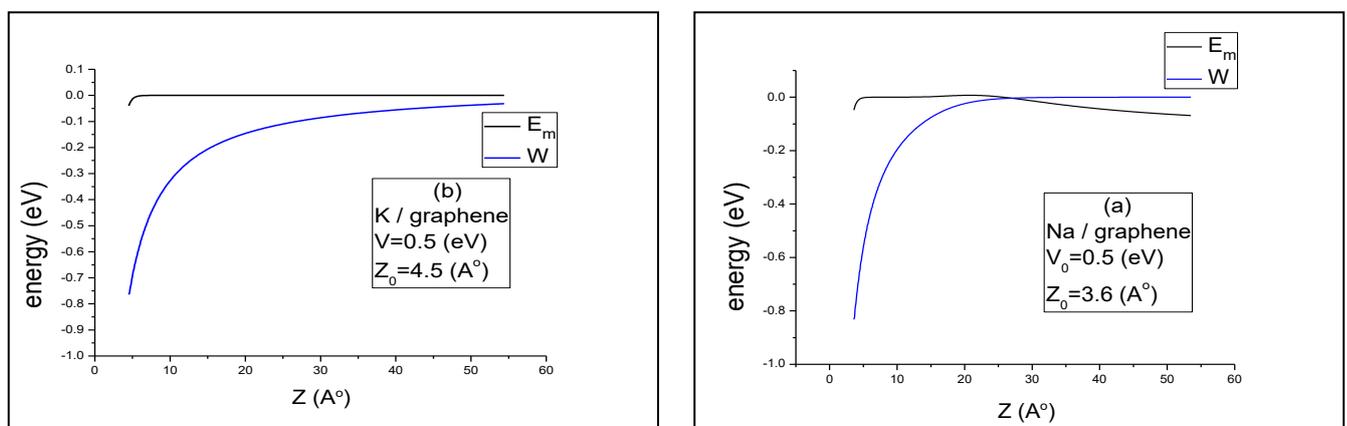


Fig. (10): The metallic and ionic portions of the chemisorption energy as a function of Z for the alkali atoms/graphene system.

Table (3) : The metallic and the ionic portions of the chemisorption energy for the alkali/graphene system at $Z=Z_0$ with $V_0=0.5$ (eV) .

Atom	Na	K
$\emptyset-V_i$ (eV)	-0.14	0.66
Z_0 (A°)	3.6	4.5
$E_m(Z_0)$ (eV)	-0.04829	-0.0401
$W(Z_0)$ (eV)	-0.8319	-0.76437
E_{bonding} (eV)[17]	-0.7	-0.8
E_{bonding} (eV) in our work	-0.74019	-0.80447

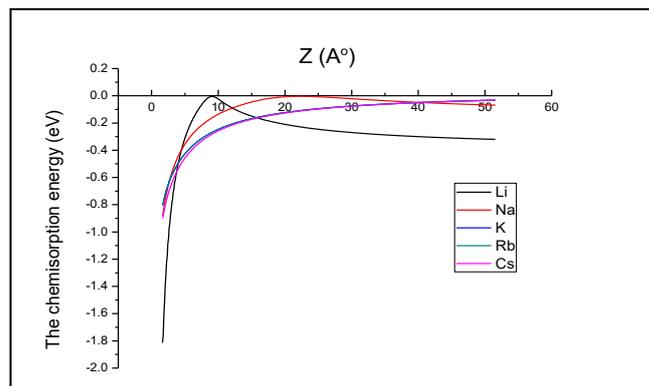


Fig.(11):The total chemisorption energy for the alkali atoms as a function of distance.

Finally, the density of states of the imperfect graphene can be easily calculated for the adatom/graphene system by using the following equation :

$\rho_{im}(E) = \rho_{ad}^\sigma(E) + \rho_{ad}^{-\sigma}(E) + \rho_G(E)$ The density of states of the imperfect graphene is calculated for alkali atom/graphene systems (fig. (12)) at $Z=Z_0$.

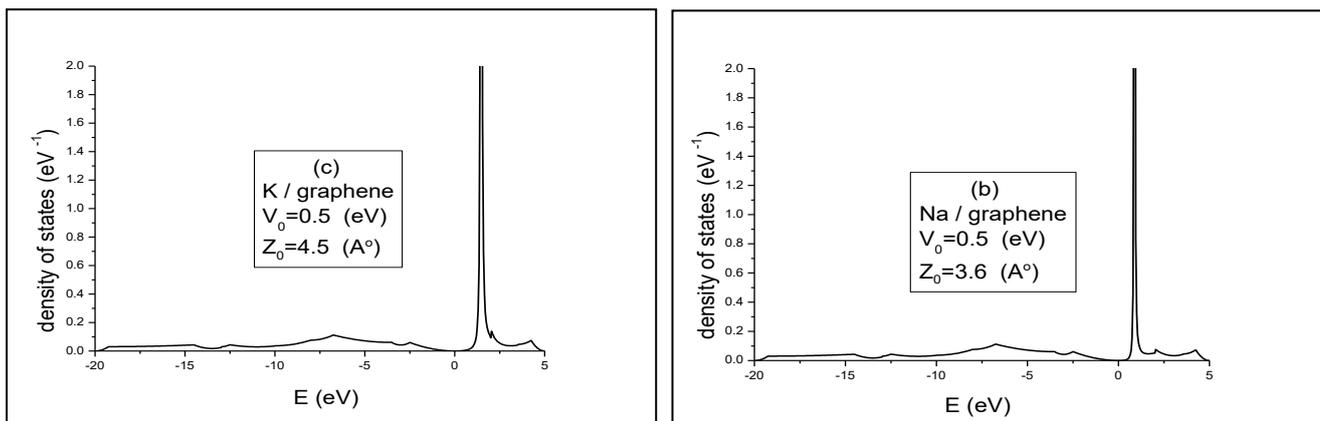


Fig. (12): The density of states of the imperfect graphene for the alkali atom/graphene systems.

The Conclusions

The Magnetic and Nonmagnetic Solutions: The self-consistent solution for Na atom at relatively large distance is magnetic, then at certain distance ($Z=Z_{ch}$) the solution is changed to nonmagnetic one. While for the K atom, the solution is nonmagnetic for all distances. The value of Z_{ch} for Na atom is $14.3001A^\circ$. The value of Z_{ch} for Na atom can be controlled experimentally by several effects such as the effect of magnetic field on the atom.

As n_a^σ is equal to $n_a^{-\sigma}$ the state of alkali's atoms is nonmagnetic, i.e. there is no net spin on the adsorbed atom, the magnetization is zero.

The Chemisorption Energy: Our calculations show that the alkali adatoms chemisorption on graphene release their valance electron easily and act as good agents for n-doping of graphene. Therefore the interaction between alkali adatoms and graphene is mainly ionic.

This confirms that the metallic chemisorption energy is vanished. The ionic energy is the dominant one for all Z values, which gives the obvious description to the type of bonding formed with the graphene.

Notably, we use the perfect density of states in our calculation. However, another formulism, presented will be in the next future work for the deformed graphene sheet that is useful for investigating the mechanical properties of the system under consideration.

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دراسة نظرية في الالتصاق الكيميائي للذرات القلوية على شريحة الكرافين*

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المستخلص

استخدمنا نموذج نيونز - اندرسون لدراسة الالتصاق الكيميائي للذرات القلوية (الصوديوم و البوتاسيوم) على الكرافين التام. الحل التوافقي الذاتي لمستويات اشغال الذرات القلوية يبين أن الحل الفيزيائي (لذرة البوتاسيوم) هو غير مغناطيسي لكل قيم المسافة الاعتيادية من شريحة الكرافين ، بينما لذرة الصوديوم ، فإن الحل غير مغناطيسي عند المسافات الصغيرة ومغناطيسياً عند المسافات الكبيرة نسبياً. وفقاً لذلك ، نوع التمغظ يحدد الجزء السائد من طاقة الالتصاق الكيميائي على الذرة الملتصقة. الجزء الأيوني من طاقة الالتصاق الكيميائي هو السائد عند شريحة الكرافين ، والذي يعطي وصفاً واضحاً عن نوع التآصر للذرات القلوية مع الكرافين.

الكلمات المفتاحية: كرافين ، التصاق كيميائي ، تمغظ ، نانوتكنولوجي .

• جزء من اطروحة دكتوراه للباحث الاول

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