

**The effects of Na & Mg adsorption on the electrical properties of Si CNTs:  
A DFT study**

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**ABSTRACT**

In the present study we focused on the electronic and structural properties of Na and Mg adsorption on the surface of the (6, 6) armchair Si CNTs. The adsorption energy ( $E_{ads}$ ), band gap energy ( $E_g$ ), partial density of state (PDOS), chemical potential ( $\mu$ ), global hardness ( $\eta$ ), electrophilicity index ( $\omega$ ), global softness ( $S$ ), work function values ( $\phi$ ) and work function change ( $\Delta\phi$ ) are calculated by using DFT methods and B3LYP/6-311++G (d, p) level of theory. Adsorption of Na and Mg atoms on the surface of Si CNTs reduce the gap energy ( $E_g$ ) of nanotube and so the conductivity and chemical reactivity of nanotube/Na or Mg increase significantly from pristine model. The order of decreasing of the  $E_g$  values for the studied systems is: Si CNTs > C-Si C/Mg > Si-Si C/Mg > C-Si C/Na > Si-Si C/Na. On the other hand the work function of the Si CNTs/Na or Mg complex alters significantly from pristine model and consequently the field emission current densities of system enhance. The predicted adsorption energies ( $E_{ads}$ ) follow the order: Si-Si C/Mg > Si-Si C/Na > C-Si C/Mg > C-Si C/Na.

**Keywords:** SiCNTs; DFT; Na & Mg Adsorption; Quantum parameters

**1. INTRODUCTION**

<sup>1</sup> The existence of tubular forms of matter with Nano scale diameters has opened an exciting field of research in science. Carbon nanotube (CNT) as a novel nano-material has been the center of attention during the past decade [1]. Owing to their unique quasi-one-dimensional atomic structure and superb mechanical and electronic properties, the CNT has been playing a significant role in emerging nanotechnology [2–4]. Purification or controlled synthesis of CNTs with selected

helicity has not been achieved so far which has made the manufacturing of electronic devices with CNTs difficult. It has been shown that the CNTs can be either metal or semiconductor depending upon the tube diameter and chirality [5]. Its high aspect ratio leads to a large electric field enhancement and a low emission threshold voltage. In recent years, much research interest has been focused on the synthesis of other kinds of quasi-one-dimensional nanotubes. Scientists have started to study

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other group IV element-based nanotubes, such as silicon carbide nanotubes (Si CNTs) due to their novel electronic properties and promising applications in building nano devices. Unlike carbon nanotubes, the Si C ones exhibit semiconductor behavior independently of its chirality [6]. Tuning the electronic structures of the semiconducting Si CNTs for specific application is evidently important in building nano scale electronic devices. Gas molecular adsorption in graphene and nanotubes is an important issue for both fundamental research and technical application. For example, the adsorption of gas molecules on nanotubes has the considerable potential for applications in fuel cells, gas sensors, and hydrogen storages [7–11]. Nanotubes are porous materials with high reactivity of exterior surface which makes them sensitive to molecular adsorption. So far, many different aspects of adsorbate/nanotube have been experimentally and theoretically explored. The reactivity of these nanotubes is often adjusted by doping with other elements. Zhao and Ding [12], theoretically demonstrated that the conductance of pure SiCNTs could be dramatically altered when exposed to CO<sub>2</sub> gas. In the recent years many researches have been done to exploring Co, Mo, Fe, Ni and Cu metals encapsulated inside nanotube for detecting electrical properties of nanotube [13–18].

Beheshtian et al. studied the adsorption of three metals Na, Mg, and Al on the surface of BN nanotubes (BNNT). Their results demonstrated that the metal adsorption decreased the energy gap and resulting in enhanced electrical conductivity of nanotube [19].

After our previous study [20–22], here in lies our motivation for optimizing structures, calculating the adsorption energy of Na and Mg atoms on the surfaces of Si CNTs. The interaction may

change the electrical and conducting properties of the nanotube. The obtained results may provide a new insight into the electronic devices and sensor applications. To our best of knowledge, there is no theoretical study reported on the Na & Mg adsorbed Si C nanotube.

## 2. COMPUTATIONAL DETAILS

In this research, the adsorption behavior of the Na and Mg atoms on the surface of Si and C atoms of (6,6) armchair Si CNTs with 156 Si and C atoms are investigated theoretically using Gaussian 03 program package [23], and density functional theory (DFT) with B3LYP/6-311++G (d, p) level of theory. The adsorption energy ( $E_{ads}$ ) of Na and Mg atoms on the pristine (6, 6) armchair Si CNTs are calculated as follows:

$$E_{ads} = E(A) - E(B) - E(C) \quad (1)$$

where  $E(A)$  is the total energy of SiCNTs/Na or Mg,  $E(B)$  and  $E(C)$  are the total energy of optimized pristine Si CNTs and the total energy of isolated Na and Mg atoms, respectively. Finally from the optimized structures, the chemical potential ( $\mu$ ), global hardness ( $\eta$ ), electrophilicity index ( $\omega$ ), global softness ( $S$ ), electro negativity ( $\chi$ ), work function values ( $\phi$ ), work function change ( $\Delta\phi$ ) of the nanotubes are calculated. In an N-electron system having total energy of  $E$  and external potential of  $v(r)$  the chemical potential ( $\mu$ ) is given by [24]:

$$\mu = \left( \frac{\partial E}{\partial N} \right)_{v(r)} \quad (2)$$

where  $\mu$  is the chemical potential of the species which is defined as the negative of electronegativity ( $\chi$ ). Similarly the global hardness ( $\eta$ ) is expressed in terms of the second derivative of energy with respect to the external potential  $v(r)$  and is given by [24]:

$$\eta = \left( \frac{\partial^2 E}{\partial N^2} \right)_{v(r)} \quad (3)$$

In finite difference approach, chemical potential and global hardness can be approximated as [25]:

$$\mu = \left( \frac{E_{HOMO} - E_{LUMO}}{2} \right) = \left( \frac{-(I + A)}{2} \right) \quad (4)$$

$$\eta = \left( \frac{I - A}{2} \right) \quad (5)$$

where  $I$  is the ionization potential and  $A$  is the electron affinity of the molecule [25]. The Frontier orbital approach as proposed by Koopmans's theorem [26, 27], for closed shell systems is very appropriate in explaining stability and chemical reactivity of molecules based on HOMO and LUMO orbital's. The energy corresponding to HOMO represents the ionization potential of the molecule while the one corresponding to LUMO represents the electron affinity value. Using the Koopmans' theorem,  $I$  and  $A$  values can be correlated with the Frontier orbitals by the following relation [26]:

$$I = -E_{HOMO} \quad (6)$$

$$A = -E_{LUMO} \quad (7)$$

The band gap energy ( $E_g$ ), electrophilicity index ( $\omega$ ) and global softness ( $S$ ) [28–30] are defined as following equations, respectively.

$$E_g = E_{LUMO} - E_{HOMO} \quad (8)$$

$$s = \frac{1}{2\eta} \quad (9)$$

$$\omega = \frac{\mu^2}{2\eta} = \frac{\left( \frac{I + A}{2} \right)^2}{(I - A)} \quad (10)$$

The maximum amount of electronic charge,  $\Delta N_{\max}$ , that the electrophone system may accept is given by **Eq. (11)** as [25].

$$\Delta N_{\max} = -\frac{\mu}{\eta} \quad (11)$$

Thus, while the quantity of  $\omega$  illustrates the tendency of the system to obtain additional electronic charge from the environment, the quantity of  $\Delta N_{\max}$  describes the charge capacity of the molecule [25].

### 3. RESULTS AND DISCUSSIONS

The optimized structures, geometrical parameters Si CNTs studied in the present work, have been shown in Fig. 1 (A, B). As seen, the optimized diameter for the (6, 6) armchair Si CNTs found to be 10.5012 Å. Essentially, for the single wall Si CNTs, two types of Si-C bonds can be observed: one type is in parallel with the tube axis and another that are not in parallel with the tube axis (diagonal bond). The calculated values of parallel bonds and diagonal bonds of (6, 6) armchair Si CNTs are found to be 1.7956 Å. For each nanotube, the Na and Mg atoms are placed outside of tube and the configurations are denoted by A and B Symbols respectively. The calculated results of geometrical parameters of pristine Si CNTs have been indicated in Table 1.

In order to investigate the interaction between Na and Mg atoms with pristine Si CNTs system, we have probed a number of different adsorption sites on the tube surface including above the Si and C atoms, and for Si\C bonds as well as above the center of a hexagonal ring in order to find the stable configurations (local minima) for the metal/Si CNTs system.

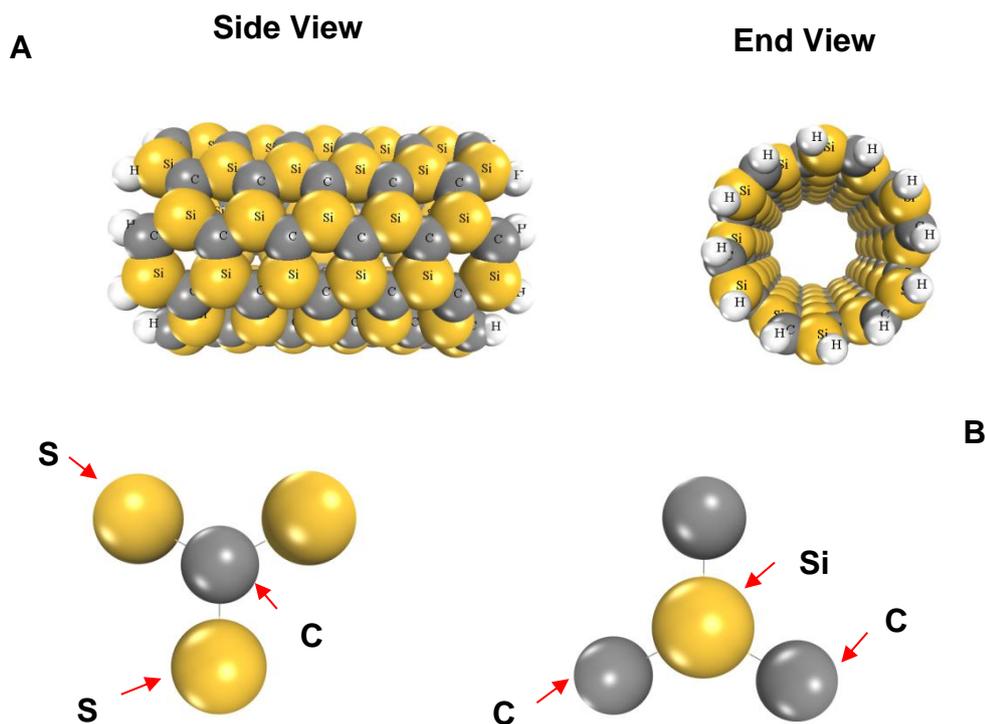
Full structural relax optimization has been performed with each initial atom-cluster distance. After full optimization four stable models considered for this study: the  $Q_1$  and  $Q_2$  symbols are used to identify a Na adsorption on the C and Si surface of nanotube; the  $Q_3$  and  $Q_4$

symbols are used to reveal a Mg adsorption on the C and Si surface of nanotube.

The  $E_{ads}$  values of the Q<sub>1</sub>, Q<sub>2</sub>, Q<sub>3</sub>, and Q<sub>4</sub> models are calculated according to the Eq. (1). A positive or negative value in  $E_{ads}$

refers to an endothermic or exothermic adsorption, respectively.

The interaction models are displayed in Fig. 2. including directions and distance between Na or Mg atoms with nanotube surface.

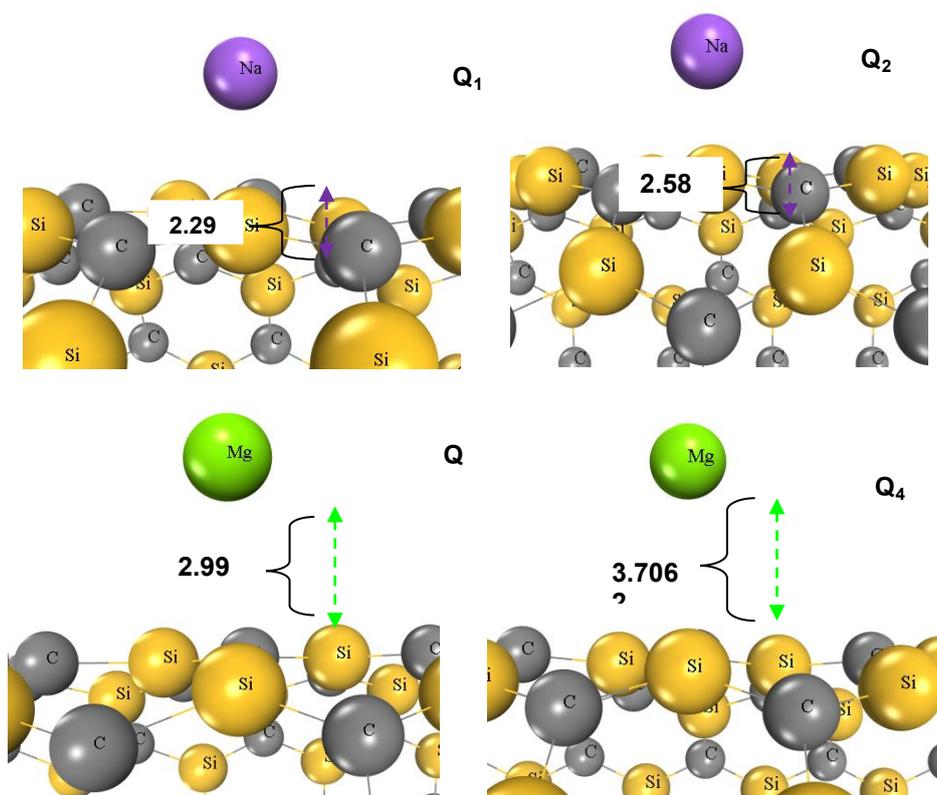


**Fig. 1.** Optimized structures of the pristine SiCNTs and B and C are the adsorption position.

**Table 1** Adsorption energy of Na and Mg atoms on the pristine Si CNTs, ( $E_{ads}$ ) (kcal/mol), HOMO energies ( $E_{HOMO}$ ) (eV), LUMO energies ( $E_{LUMO}$ ) (eV), HOMO-LUMO energy gap ( $E_g$ ) (eV), Distance (Å) Between the Na, and Mg atoms and nearest atom (C or Si) of the pristine Si CNTs, Fermi level ( $E_F$ ) (eV), work function values ( $\Phi$ ), work function change ( $\Delta\Phi$ ) (eV) for the Si CNTs, Si CNTs/Na, Mg system

Property	Model	$E_{HOMO}$	$E_{LUMO}$	$E_g$	$E_F$	$E_{ads}$	Distance	$\Phi$	$\Delta\Phi^a$
SiCNTs	A	-5.2243	-1.8503	3.3740	-3.5373	-	-	3.5373	-
C-SiCNTs/Na	Q <sub>1</sub>	-3.6734	-2.0680	1.6054	-2.8707	1.3258	2.5807	2.8707	-0.6666
Si-SiCNTs/Na	Q <sub>2</sub>	-2.8843	-1.8503	1.0340	-2.3673	17.3193	2.2998	2.3673	-1.1700
C-SiCNTs/Mg	Q <sub>3</sub>	-5.0883	-2.1768	2.9115	-3.6325	1.6943	3.7062	3.6325	0.0952
Si-SiCNTs/Mg	Q <sub>4</sub>	-4.1903	-1.9863	2.2040	-3.0883	25.8534	2.9998	3.0883	-0.4490

<sup>a</sup> work function changes of the C, Si-Si CNTs after the adsorption of Na and Mg atoms.



**Fig. 2.** Optimized structures of a Na and Mg atoms adsorbed on the pristine Si CNTs. Q<sub>1</sub> and Q<sub>3</sub> models denote Na and Mg atoms closed to C site of pristine Si CNTs respectively, the Q<sub>2</sub> and Q<sub>4</sub> models denote Na and Mg atoms closed to Si site of pristine Si CNTs, respectively.

As we can see in Fig. 2, when a Na and Mg atoms adsorbed on the Si CNTs surface, the  $E_{ads}$  values for Q<sub>1</sub>, Q<sub>2</sub>, Q<sub>3</sub> and Q<sub>4</sub> models are 1.3258, 17.3193, 1.6943 and 25.8534 eV respectively. On the other hand the distance between Na and Mg atoms with nanotube surface for the Q<sub>1</sub>, Q<sub>2</sub>, Q<sub>3</sub> and Q<sub>4</sub> models are 2.5807, 2.2998, 3.7063 and 2.9998 Å respectively (see Table 1). The positive values of adsorption energy indicated that the adsorption process of Na and Mg on the surface of nanotube is endothermic in thermodynamic approach. The order of adsorption energy for the Q<sub>1</sub>, Q<sub>2</sub>, Q<sub>3</sub> and Q<sub>4</sub> models are: Q<sub>4</sub> > Q<sub>2</sub> > Q<sub>3</sub> > Q<sub>1</sub>. Inspection of results demonstrates that the interaction of Na and Mg on the Si site of nanotube (Q<sub>2</sub> and Q<sub>4</sub> models) are stronger than Na and Mg on the C site of nanotube. The small  $E_{ads}$

values and large interaction distance in the Q<sub>1</sub> and Q<sub>3</sub> indicate that the adsorption of Na and Mg atoms on the C site of nanotube is weakly physical adsorption due to weak Vander Waals interaction between the nanotube and Na and Mg atoms.

However, one of the most important characteristics for making sensors is the recovery time. The stronger interaction simply that desorption of the adsorbate could be difficult and the device may suffer from long recovery times. If  $E_{ads}$  is significantly increased, much longer recovery time is expected. Based on the conventional transition state theory, the recovery time,  $\tau$ , can be expressed as:

$$\tau = \nu_0^{-1} \exp\left(\frac{-E_{ads}}{kT}\right) \quad (12)$$

Where  $T$  is the temperature,  $k$  is Boltzmann's constant and  $\nu_0$  is the attempt frequency. According to this equation, more negative  $E_{\text{ads}}$  value will prolong the recovery time in an exponential manner. However, as an advantage the adsorption energies of Na and Mg atoms are not large enough to hinder the recovery of pristine Si CNTs and the recovery time may be large according to Eq. (12).

Comparisons the obtained results reveal that the  $E_{\text{ads}}$  values of Mg atom on Si CNTs are higher than that of Na atom. This observation may be rationalized based on Pearson's hard-soft acid-base theory (HSAB), which states that the soft acids react strongly with the soft bases and in contrary, the hard acids react strongly with the hard bases, when all other factors being equal. The Mg atom for Si CNTs is a hard acid with smaller size, therefore, it tends to interact more referable with nitrogen which is known as a hard acid, in comparison with Na and Mg atoms.

One of the most important parameters for electrical analysis of system is the band gap energy ( $E_g$ ). The  $E_g$  value is equivalent to the energy required to release an outer shell electron from its orbit about the nucleus to act as a mobile charge carrier, able to move freely within the material. So the  $E_g$  is a major factor determining the electrical conductivity of a material and the classic relation between them is as follows:

$$\sigma \propto \exp\left[-\frac{E_g}{2kT}\right] \quad (13)$$

where  $\sigma$  is the electrical conductivity and  $k$  is the Boltzmann constant. According to the equation 13, smaller values of  $E_g$  at a given temperature lead to larger electric conductivity. In order to further analysis the conductivity properties of nanotube, we study the electronic band structure near the Fermi level for the Na and Mg atoms closed to the pristine Si CNTs. As seen in

Table 1, with adsorbing Na and Mg atoms the  $E_g$  of Si CNTs decrease significantly from 3.3740 to 1.0340 and 2.2040 eV respectively. The order of decreasing of the  $E_g$  values for the studied systems is: Si CNTs > Q<sub>3</sub> > Q<sub>4</sub> > Q<sub>1</sub> > Q<sub>2</sub>. Comparison results indicate that with adsorbing Na atom on the Si site of nanotube (Q<sub>2</sub> models) the  $E_g$  value is lower than the other those models and also the conductivity of nanotube is more than the other those models. Thereby this model is more favorable than those models for making electronic device and micro sensors applications.

On the other hand these calculations demonstrate that the Na and Mg atoms acts as an electron donor and the nanotubes act as an electron acceptor in the adsorption processes. Clearly, when Na and Mg atoms are closed to the C, Si-Si CNTs, A new heterozygous state is generated in the near bottom of the conduction band and the top of the valence band and so the band gap is narrowed obviously near the Fermi level. This effect enhances the conductive ability of the nanotube with Na and Mg atoms adsorption.

Meanwhile, to investigate the sensitivity of pristine Si CNTs further, we have studied  $\Delta\phi$  of systems ascribed to the charge transfer between Na and Mg atoms and the adsorbents. The  $\phi$  of a semiconductor is the least amount of energy required to remove an electron from the Fermi level to a point far enough not to feel any influence from the material. The change of work function of an adsorbent after the gas adsorption alters its field emission properties. The readout of gas-induced  $\Delta\phi$  via suspended gate field effect devices and has been accepted as a promising technique for the realization of a sensor platform for several years [31]. However, the emitted electron current densities in vacuum are theoretically

described by the following classical equation:

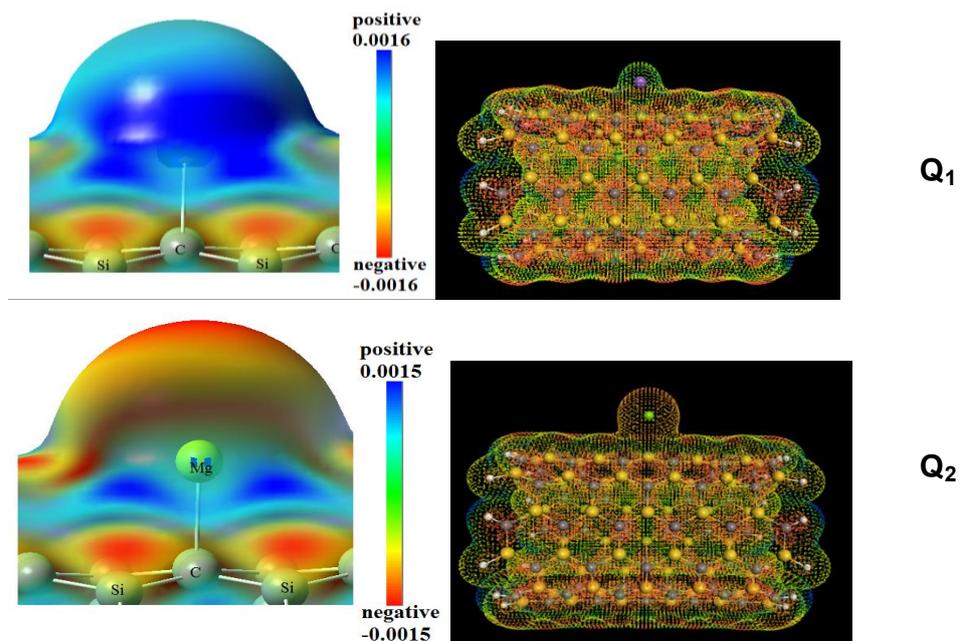
$$j = AT^2 \exp\left[-\frac{\phi}{kT}\right] \quad (14)$$

where  $A$  is called the Richardson constant ( $A/m^2$ ),  $T$  is the temperature (K) and  $\phi$  (eV) is the material's work function. Work function values were calculated using the following equation:

$$\phi = E_{\text{inf}} - E_F \quad (15)$$

where  $E_{\text{inf}}$  the electrostatic potential at infinity and  $E_F$  is the Fermi level energy. The electrostatic potential at infinity is assumed to be zero. The  $\Delta\phi$  was calculated by subtracting the  $\phi$  of pristine Si CNTs from that of the corresponding adsorbed system. The results of Table 1 reveal that calculated work function of the pristine Si CNTs are about 3.53 eV for the pristine which does not significantly change after the adsorption of Na and Mg atoms. Interestingly, after the adsorption of Na

and Mg atoms at the  $Q_2$  and  $Q_4$  models the work function is decreased considerably from 3.5373 to 2.3673 and 3.0883 eV respectively. A negative work function change may arise from a donation of charge from the Na and Mg atoms to the nanotubes surface which correlates with an increase in the nano tubes conductance after exposure to the target adsorb ate, as has been shown before. However, as can be seen from Eq. (14), the emitted electron current density is exponentially related with the negative value of  $\phi$ . The emitted electron current density from the pristine Si CNTs will be significantly decreased after the adsorption of Na and Mg atoms. Consequently the Na and Mg adsorption can be regarded as a good strategy to improve the sensitivity and conductivity of Si CNTs. To further study, the molecular electrostatic potential (MEP) maps for Na and Mg adsorption models are calculated, and results are shown in Fig. 3. The graphical results indicate that the positive

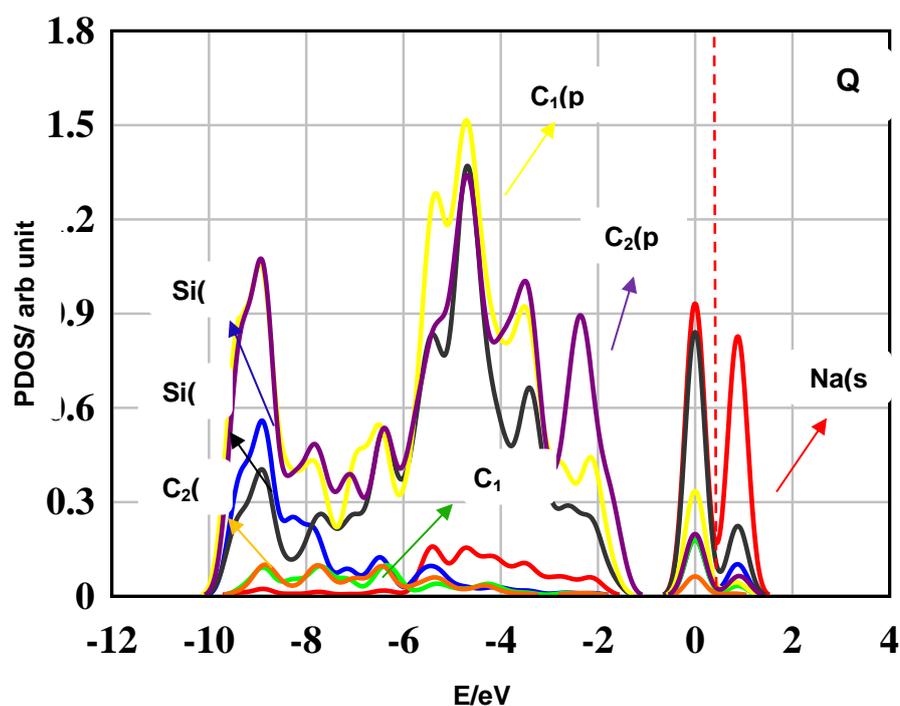
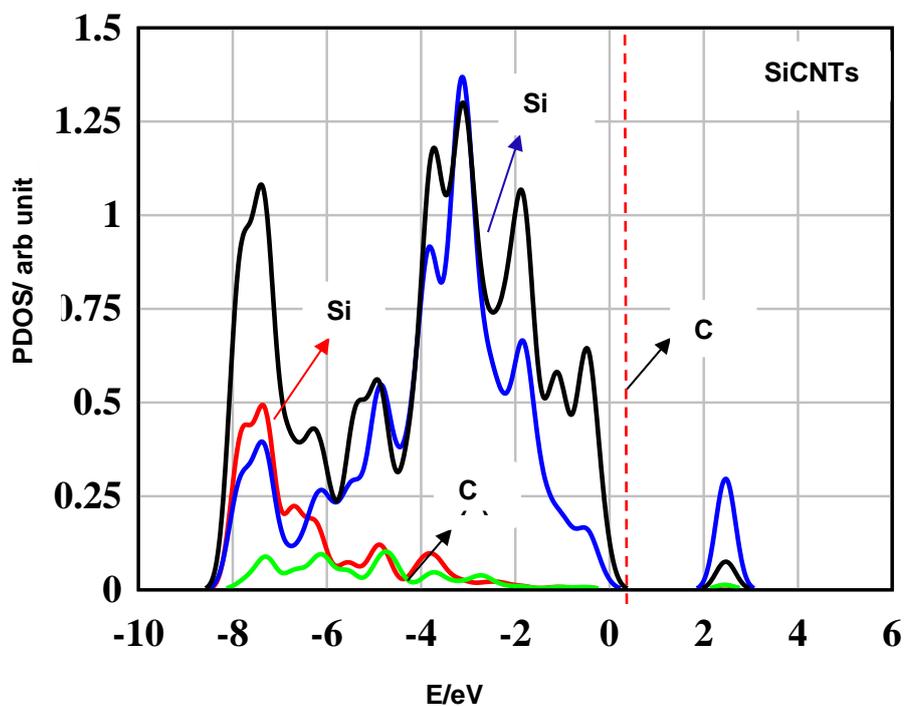


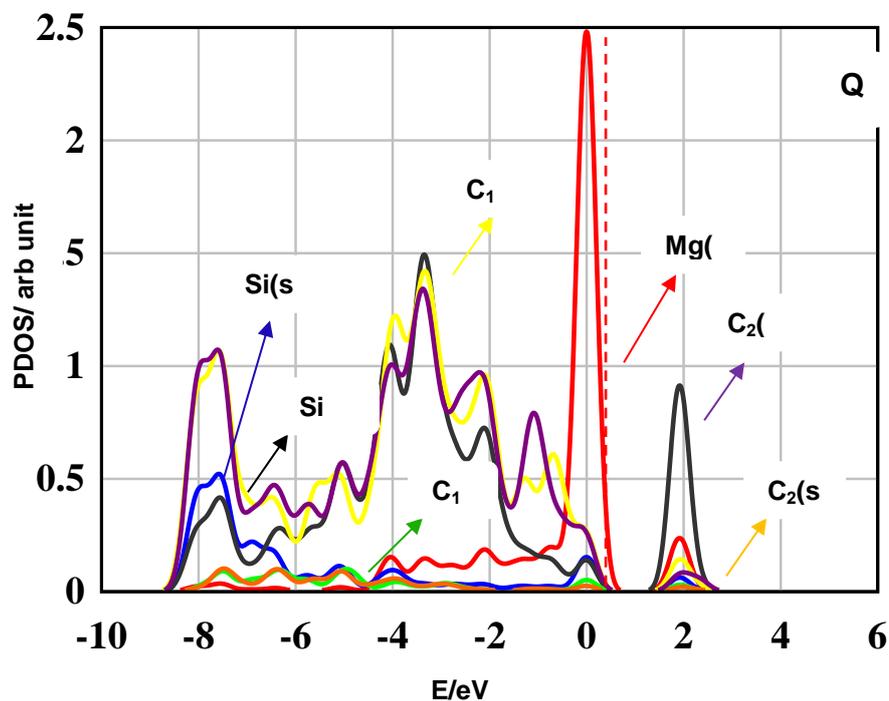
**Fig. 3.** Totalelectron density of Na and Mg atoms adsorption on surfaces SiCNTs for  $Q_1$  and  $Q_3$  model (see Fig. 2).

electron donor (blue color) and the nano tubes acts as an electron acceptor (red color)

Furthermore, for study the influence effects of Na and Mg atoms adsorption on

the electronic properties of the complexes, the partial densities of states (PDOS) are calculated and results are shown in Fig. 4.





**Fig. 4** Partial density of state (PDOSs) for Na, Mg, Si and C atoms of pristine,  $Q_2$  and  $Q_4$  models (see Fig. 2).

These results showed that when the pristine Si CNTs models are under interaction with Na and Mg atoms, the stronger interaction is observed for  $Q_2$  and  $Q_4$  models and the lower interaction is perceived for  $Q_1$  and  $Q_3$  models. In Fig. 4,  $M_1$ ,  $M_2$  and  $M_3$  symbols are used to depict the PDOSs of the Na, Si and C atoms in the pristine Si CNTs, Na and Mg atoms adsorbed on the Si-Si CNTs systems ( $Q_2$  and  $Q_4$  models) respectively. For this purpose, the s orbitals of Na and Mg atoms, the p orbitals of Si and C around the Fermi level are plotted in Fig. 4. As we can see, the PDOS of all models are significantly changed when the Na and Mg atoms adsorbed on the Si CNTs surface. Comparison results reveal that, in the  $Q_2$  model ( $M_2$  symbol), the s orbital of Na have a small effectively overlap with the p orbitals of C atom around the Fermi level, and consequently the Na atom cannot strongly hybridize with C atom. While in

the  $Q_4$  model ( $M_3$  symbol) the s orbital of Mg atom have a large effectively overlap with the p orbitals of Si atom around the Fermi level, and therefore the Mg atom can strongly hybridize with Si atom. Thereby the position of the local energy levels of Si atom has been changed with adsorbing of the Mg atom. This finding could provide a useful guide for exploring new applications of Si CNTs in nano devices such as sensors for Na and Mg atoms.

To facilitate a more extensive understanding of the interaction of Na and Mg adsorption on Si CNTs the HOMO and LUMO energies are calculated and results are plotted in Fig. 5. As can be seen from Fig. 5, the HOMO energy of  $Q_1$  and  $Q_2$  models (Na adsorption) increase significantly from pristine Si CNTs, on the other hand the HOMO energy of  $Q_3$  and  $Q_4$  models (Mg adsorption) increase slightly from original values, this result demonstrate that the Na and Mg are

nucleophile agent and increase density of electron on the surface of nanotube.

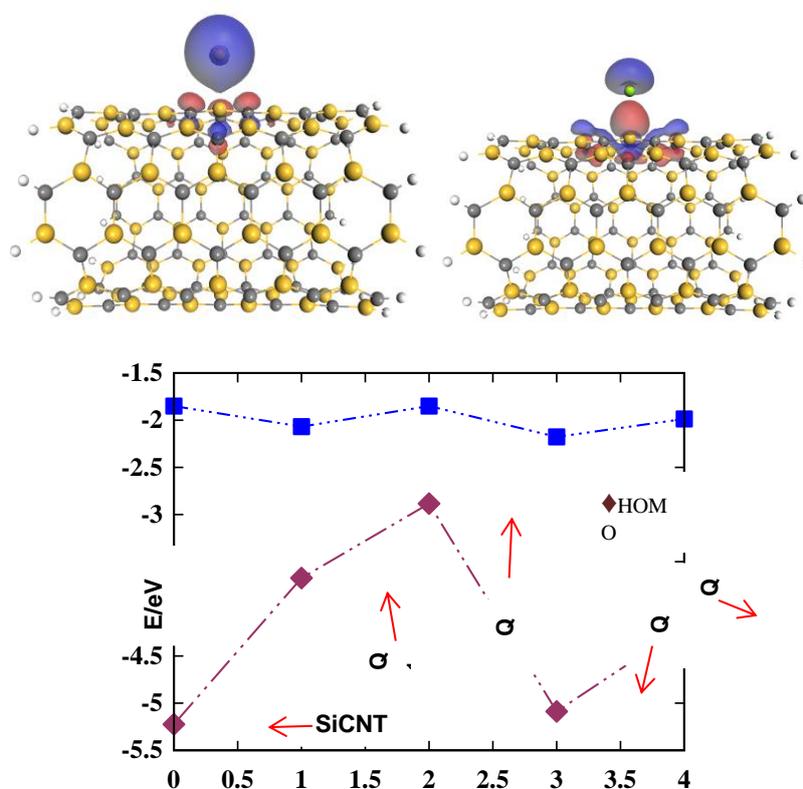
It is interesting that the small values of  $E_{\text{ads}}$  values for the Q<sub>1</sub> and Q<sub>3</sub> models may be depended to higher differences between HOMO and LUMO energy. For this means the interaction between Na and Mg atoms at the C site of nanotube is very weak and the adsorption energy is lower than other those models.

The global hardness ( $\eta$ ), the maximum amount of electronic charge ( $\Delta N_{\text{max}}$ ), electrophilicity index ( $\omega$ ), the chemical potential ( $\mu$ ) and global softness ( $S$ ) in the context of the DFT for the most stable configuration of Na and Mg atom introducing Si CNTs are presented in Table 2.

Since the global hardness of a species is defined as its resistance towards deformation in presence of an electric

field, increase in global hardness leads to increase in stability and decrease in reactivity of the species [32–33]. When Na and Mg atoms are adsorbed on surface of Si CNTs, with decreasing  $E_g$  values the global hardness and electrophilicity of all models decrease significantly from original values and so the reactivity of system increase from original values.

On the other hand the positive values of the  $\Delta N_{\text{max}}$  and  $\omega$  for Q<sub>1</sub>, Q<sub>2</sub>, Q<sub>3</sub> and Q<sub>4</sub> models reveal that the tendency of the Si CNTs to obtain additional electronic charge from the Na and Mg atoms and so the charge capacity of the nanotube/Na & Mg complex is more than pristine model. Comparing results show that the  $\mu$  values of the Q<sub>1</sub>, Q<sub>2</sub> and Q<sub>4</sub> models are lower than the pristine model and the  $\mu$  value of the Q<sub>3</sub> model is more than other those models.



**Fig. 5.** HOMO-LUMO plot and graph of HOMO and LUMO energy of the pristine, Q<sub>1</sub>, Q<sub>2</sub>, Q<sub>3</sub> and Q<sub>4</sub> models (see Fig. 2).

**Table 2.** Chemical Potential ( $\mu$ ) (eV), hardness ( $\eta$ ) (eV), softness ( $S$ ) ( $\text{eV}^{-1}$ ), electrophilicity ( $\omega$ ) (eV), and  $\Delta N_{\text{max}}$  (eV) Na and Mg atoms adsorption on the pristine SiCNTs Surface

Models	I	A	$\eta$	$\mu$	S	$\omega$	$N_{\text{max}}$
A	5.2243	1.8503	1.6870	3.5373	-0.2964	3.7085	1.0484
Q1	3.6734	2.0680	0.8027	2.8707	-0.6229	5.1331	1.7881
Q2	2.8843	1.8503	0.5170	2.3673	-0.9671	5.4198	2.2895
Q3	5.0883	2.1768	1.4557	3.6325	-0.3435	4.5322	1.2477
Q4	4.1903	1.9863	1.1020	3.0883	-0.4537	4.3275	1.4012

#### 4. CONCLUSION

In this article, we have systematically investigated the stability and electronic properties of the pristine Si CNTs with and without the Na and Mg atoms adsorption, using a first principles calculation based on the density functional theory. The calculated results show the adsorption process at all models is endothermic in thermodynamic approach. With introducing Na and Mg atoms the gap bond energy of system significantly reduces and so the conductivity and reactivity of system significantly increase from pristine model. The Na and Mg adsorption can be regarded as a good strategy to improve the sensitivity and conductivity of Si CNTs. Comparison results reveal that the  $E_g$  value of the Q<sub>2</sub> model is lower than the other those models and also the conductivity of this model is more than the other those models. Consequently the Q<sub>2</sub> model is more favorable than those models for making electronic device and micro sensors applications.

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