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Electric Field Effect in CO Adsorption on the (6,0) Zigzag Single-walled Aluminum Nitride Nanotube: an Ideal Method for CO Adsorption

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The behavior of the monoxide carbon (CO) adsorbed on the external surface of H-capped (6,0) *zigzag* single-walled aluminum nitride nanotube was studied under the parallel and transverse electric fields with strengths 0-140 × 10^{-4} a.u. by using density functional calculations. Geometry optimizations were carried out at the B3LYP/6-31G* level of theory using the Gaussian 03 suite of programs. The binding energies obtained from these calculations at different applied parallel and transverse electric field strengths indicate that with increasing parallel electric field intensity, the binding energy values are increased, especially in the higher parallel field strength, whereas the *BE* values for the applied transverse electric field show a significant reverse trend. Results of this study indicate that with increasing parallel electric field intensity the pristine AlNNT can be used as CO storage and the parallel electric field effect is an ideal method for adsorption, storage, and fabrication of CO sensors.

Keywords: Aluminum nitride nanotube, Adsorption, Dipole moment.

PACS numbers: 68.43. – h, 61.46.Fg

1. INTRODUCTION

Tuning the electronic structures of the semiconducting AlNNTs for specific application is evident important in building specific electronic and mechanical devices. Improving the sensing performance of the pristine nanotubes and nano sheets by manipulating their structure is too expensive; therefore, finding high sensitive pristine nanotubes is of scientific interest. Electric field effect is one of the best techniques for improvement of the electronic structure properties of nanotubes and adsorption of gaseous molecules on the tubes surface. In recent years, several studies have been put in the computational calculation of the field effects on the electronic and structural properties of nanotubes [1-3]. However, to our knowledge, no experiments and theoretical investigation have been reported on adsorption of CO on AlNNT surfaces under electric field effect. Therefore, the understanding of the chemisorptions of CO on AlNNT surfaces under electric field effect is important for CO storage and fabrication of CO sensors.

2. COMPUTATIONAL METHODS

The hydrogenated models of the pristine (6,0) *zigzag* AlNNT and the CO- attached (6,0)AlNNT models consist of 72 atoms with formulas $Al_{30}N_{30}H_{16}$ (pristine), and 74 atoms with formula of $Al_{30}N_{30}H_{16}CO$. In the first step, all the atomic geometrical parameters of the structures were allowed to relax in the optimization at the DFT level of B3LYP exchange functional and 6-31G* standard basis set. The binding energy (*BE*) of the CO- attached (6,0)AlNNT complex was calculated as follows:

$$BE = [E_{\text{CO-AlNNT}}] - [E_{\text{AlNNT}} + E_{\text{CO}}] \quad (1)$$

Where $E_{\text{CO-AlNNT}}$ was obtained from optimization of the CO- attached (6,0)AlNNT model, E_{AlNNT} and E_{CO} are the energy of the optimized AlNNT and CO structures. A negative *BE* denotes exothermic substitute. Then, we studied influence of the static external electric field on adsorption and structural and electronic properties of the complex, separately applied at the positive X- and positive Y-directions, which is parallel and perpendicular to X and Y plane. The numerical values of static electric field strengths in X and Y directions on the CO- attached (6,0)AlNNT complex are 35 × 10^{-4}, 70 × 10^{-4}, 100 × 10^{-4}, and 140 × 10^{-4} a.u. (1 a.u. = 5.14224 × 10^{11} V/m) [4]. All the calculations were carried out by using the Gaussian 03 suite of programs [5].

3. RESULT AND DISCUSION

For the adsorption of CO on the AlNNT, we considered four possible sites (i.e., the center site, above the hexagon, the Al and N sites above the aluminum and nitrogen atoms, and the Z site above the zigzag and axial Al–N bond) with two orientation (C-down and O-down) as described in Fig. 1a, b. The notation C-down and O-down denotes a CO molecule oriented perpendicular to the surface via C and O atoms. We limited our analysis to the interaction of CO with the nanotube, outer walls. In the first step, the structures were allowed to relax by all atomic geometrical parameters in the optimization at the DFT level of B3LYP exchange-functional and 6-31G* standard basis set. After structural optimizations, it is found that CO adsorption on center, nitrogen, and Z sites are energetically unstable and are collapsed to the aluminum site, which is energetically favorable. The binding energies (*BEs*) of CO (C-down and O-down) with the equilibrium distances ($R_{Al\text{-}C}$ and $R_{Al\text{-}O}$) at the aluminum site on the zigzag configuration

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of (6,0) AlNNT are summarized in Fig. 1a, b. For the states, the *BEs* are attractive, which characterizes a chemisorption process, also, the calculated *BE* for CO in C-down (*BE* = -0.42 eV) is more than that in O-down (*BE* = -0.12 eV). Therefore, we limited static external electric field effect to the interaction of CO at the aluminum site with C-down.

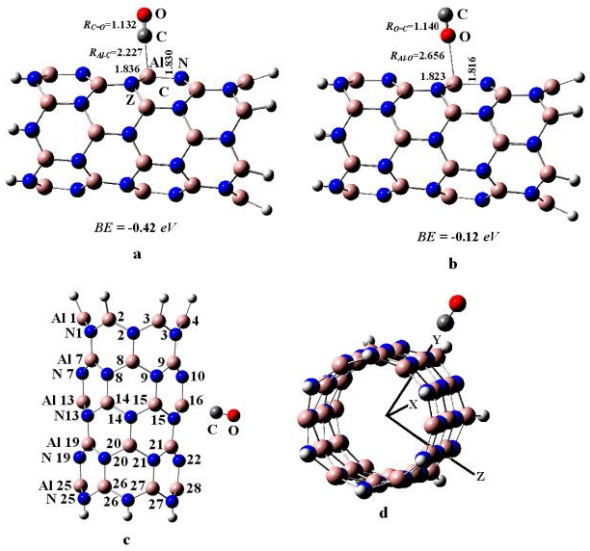

Fig. 2 – (a) and (b) Two-dimensional (2D) views and adsorption configurations of CO (C-down and O-down) on (6,0) *zigzag* AlNNT (c) 2D views of CO- attached (6,0)AlNNT complex, and (d) Three-dimensional (3D) views of the CO-attached (6,0)AlNNT complex

The total energy (E_T) and *BEs* for the optimized structure of CO-attached (6,0) AlNNT complex at the aluminum site with C-down at various applied parallel and transverse electric field strengths is calculated. The *BEs* obtained from these calculations at different applied parallel electric field strengths with respect to the corresponding values at zero fields (E_X = E_Y = 0) indicate that with increasing parallel electric field intensity, the E_T and *BE* values are increased. The *BE* values for the applied transverse electric field show a significant reverse trend, increasing with increasing transverse electric field intensity. The *BE* value for the applied parallel electric field is gradually increased from -0.42 eV at the zero field strength (E_X = 0) to – 0.80 eV at the field strength of 140 × 10^{-4} a.u (E_X = 140), whereas the *BE* value for the applied transverse electric field is gradually decreased from -0.42 eV at the zero field strength (E_Y=0) to -0.40 eV at the field strength of 140 × 10^{-4} a.u (E_Y=140). Therefore, the *BE* of the CO for the applied parallel electric field (E_X) from zero field strength to 140 × 10^{-4} a.u. increases by 90 %, and the *BE* of the CO for the applied transverse electric field (E_Y) from zero field strength to 140 × 10^{-4} a.u. decreases by 5 % . Also, the values of $R_{Al\text{-}C}$ the complex decreased slightly by external electric field. The calculated *BEs* of the complex indicated that CO can significantly be adsorbed on the AlNNT by external parallel electric field (E_X) and the CO adsorption on the AlNNT is sensitive to the strength of the electric field applied to the AlNNT surface. Therefore, with this method, pristine AlNNT can be used as CO storage and increase of parallel electric field effect (E_X) is an ideal method for CO adsorption on AlNNTs and fabrication of CO sensors.

4. CONCLUSION

We studied the adsorption of CO molecule on (6,0) zigzag AlNNT at different applied parallel and transverse electric field strengths by means of density functional theory (DFT) calculations. We compared all the *BE* of CO interacting with all possible sites of adsorption on nanotube walls in several structural configurations. The calculated *BE* for CO in C-down configuration is higher than that in O-down and aluminum site is the most stable configuration. The *BEs* obtained from these calculations at different applied parallel electric field strengths with respect to the corresponding values at zero fields indicate that with increasing parallel electric field intensity, the E_T and *BE* values are increased and CO can be absorbed significantly on the AlNNT, especially to the higher parallel field strength, whereas the *BE* values for the applied transverse electric field show a significant reverse trend..

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