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Interaction of vitamins B3 and C and their radicals with (5, 0) single-walled boron nitride nanotube for use as biosensor or in drug delivery

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Abstract. Electronic properties of the covalent and noncovalent adsorption of single-walled boron nitride nanotube with vitamins B3 and C and their radicals are investigated through the density functional theory. Results show that noncovalent and covalent adsorption of vitamin B3 on BNNT could make these systems of interest for drug delivery purposes due to the possibility of easily detaching the pristine molecule from the BNNT surface. Noncovalent and covalent adsorption of vitamin C on BNNT result in modification of the electronic properties of BNNT, these results are extremely relevant in identifying the potential application of functionalized BNNT with vitamin C as nano-sensor. The present results are expected to provide useful guidance for the relevant experimental study.

Keywords. Vitamin C; vitamin B3; density functional theory; boron nitride nanotube (BNNT).

1. Introduction

The recent explosive growth of nanotechnology has caused dramatic advances in pharmacology and is revolutionizing the delivery of biologically active compounds. Development of new and efficient drug delivery systems is of fundamental importance to improve the pharmacological profiles of many classes of therapeutic molecules. Many different types of drug delivery systems are currently available. Within the family of nanomaterials, nanotubes have emerged as a new alternative and efficient tool for transporting therapeutic molecules as nanotubes can easily shuffle cargos within cellular membranes through endocytosis.[1–8] Moreover, nanotubes could act also as sensors to identify changes in the adsorbed molecules. The need for detectors with high specificity and sensitivity has directed scientists to investigate nanotubes. At many times, chemical sensors developed from nanotubes have their acts based on the electrical properties that they have to change such as their conductance, by replying chemically with other structures. Sensors made from nanotubes have fast response time at room temperature and high sensitivity due to their large surface areas to volume ratios which are important advantages for sensing applications. In particular, nanotubes can be particularly useful for detecting biological structures.[9–14]

BNNT with its outstanding thermal,[15] mechanical,[16] chemical[17] and electrical[18] properties has attracted huge attention, since its discovery in 1995. These advantageous properties make BNNT promising material for application in nano-devices, material science, bio-technology and electronic devices in certain hazardous and high temperature environments. BNNTs are also found to be nontoxic to health and environment; therefore, they are suitable for bio-medical applications.[19] Recent studies showed that BNNTs have attracted attention in the field of nanomedicine,[20] both as nanovectors for drug delivery purpose, as intracellular nanotransducers[21] and for the development of biosensors.[22–24] On the theoretical side, interaction of BNNTs with amino acids,[25] nucleobases[26] and thiazole[27] has been reported previously. These studies suggested that BNNT can be used as a smooth nanoscale channel for transporting biological molecules and nanovector for targeted drug delivery. Consequently, it is important to understand the advantages and disadvantages of functionalizations of BNNTs for increasing their biocompatibility and further their application for drug delivery and as biosensor.

On the other hand, modification of the electronic and physical properties of nanotubes by doping and

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functionalizing is an important subject for designing of the nano-devices. Functionalized nanotubes may exhibit a dramatic change with regard to the isolated nanotubes thus, functionalization is a commonly used method to enhance the electronic properties.[28] From the theoretical results, it is reported that covalent functionalizations of BNNTs by using, NH_3,[29,30] Fluorine[31] and CCl_2,[32] can effectively modify their solubility, magnetic properties and electronic structures.

Noncovalent functionalizations of BNNTs have also been extensively explored. Theoretical studies of noncovalent functionalizations of BNNTs using organic molecules,[33] nucleobases,[34] polymers,[35] various metalloporphyrins,[36] various gas molecules[37] and H_2 molecule[38] have been reported. These studies on the noncovalent functionalizations of BNNTs provide a guidance to design BNNT-based devices such as sensing devices, molecular electronics and biomedical applications.

To our knowledge, no investigations have been reported on the interaction of vitamins B3, and C and their radicals with BNNTs. With an aim of expanding the domain of BNNT for drug delivery and as biosensor, we have studied the covalent and noncovalent functionalizations of (5, 0) BNNT with vitamins B3 and C.

Interest in the theoretical study of vitamins B3 and C stems from the fact that vitamins are essential nutrients found in foods. The requirements are small but they perform specific and vital functions essential for maintaining health. Vitamin C is a water-soluble, antioxidant vitamin. It is important in forming collagen, a protein that gives structure to bones, cartilage, muscle and blood vessels. Vitamin C also aids in the absorption of iron, and helps maintain capillaries, bones and teeth. In the same view, vitamin B3 is part of the B complex of vitamins. All of the B vitamins are water-soluble, which makes it less likely for people to develop any levels of toxicity. Vitamin B3 along with the other B vitamins converts carbohydrates into sugar, which is then used to produce energy for the body. It is also vital for maintaining muscle tone, especially along the digestive tract. It is also required for the health of hair, skin, eyes, mouth, liver and nervous system. Also, the adsorption of biological molecules on nanotubes has attracted such attention during the recent years, since it is of great importance both from the fundamental and the applied point of view.[25] It is important to be able to predict the interaction between vitamins B3 and C and BNNTs with changes in electronic structure in order to determine the nature of biological-nanotube interactions, and this knowledge is also significant for understanding their biological activity as well as the potential role they can play in nanostructure construction, BNNT-based drug delivery and biosensor systems.[39]

2. Computational details

Full geometry optimizations and all calculations were performed on the (5, 0) pristine and covalent and noncovalent functionalized single-walled boron nitride nanotube (SWBNNT) with vitamins B3 and C at the spin unrestricted B3LYP/6-31G* level of the theory as implemented in Gaussian 03 suites of program.[40] The B3LYP/6-31G* is a popular approach commonly used for nanotube structures.[41–46] We considered the (5, 0) SWBNNT with a 1 nm length, 0.42 nm dimeter which consists of 20 B and 20 N atoms. Due to the absence of periodic boundary conditions in molecular calculations, it is necessary to saturate the B and N dangling bonds with hydrogen atoms. It is important to note that due to the size effects and limitations in living systems, considering small nanotubes is very important for biologically related applications.[47] Geometry optimizations were carried out until the maximum force and root-mean-square errors on all atoms were less than 0.00045 and 0.00030 Hartree/Bohr, respectively, which are the 'normal' convergence criteria setting in Gaussian 03. Analyses of the electronic properties of the BNNT–vitamin system were based on adsorption energy, the gap of highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), charge transfer (NBO charge) and density of states (DOSs).

3. Results and discussion

3.1 *Noncovalent interaction of vitamins B3 and C with (5, 0) BNNT*

Optimized structures for vitamins B3, C and pristine (5, 0) BNNT are shown in figure 1a, b and c, respectively. To model the noncovalent interaction between BNNT and vitamins B3 and C, these vitamins are located parallel to the BNNT axis. Vitamins B3 and C atoms are allowed to relax freely in all directions, to determine the stable adsorption structures. Optimized structures of the BNNT–vitamin B3 and BNNT–vitamin C complexes are shown in figure 1d and f, respectively.

From the optimized configurations, we find that adsorption of vitamin B3 on BNNT mainly arises from interaction between N atom in the tube and H atom of the hydroxyl group in vitamin B3, while the pyridine ring in vitamins B3 does not contribute towards

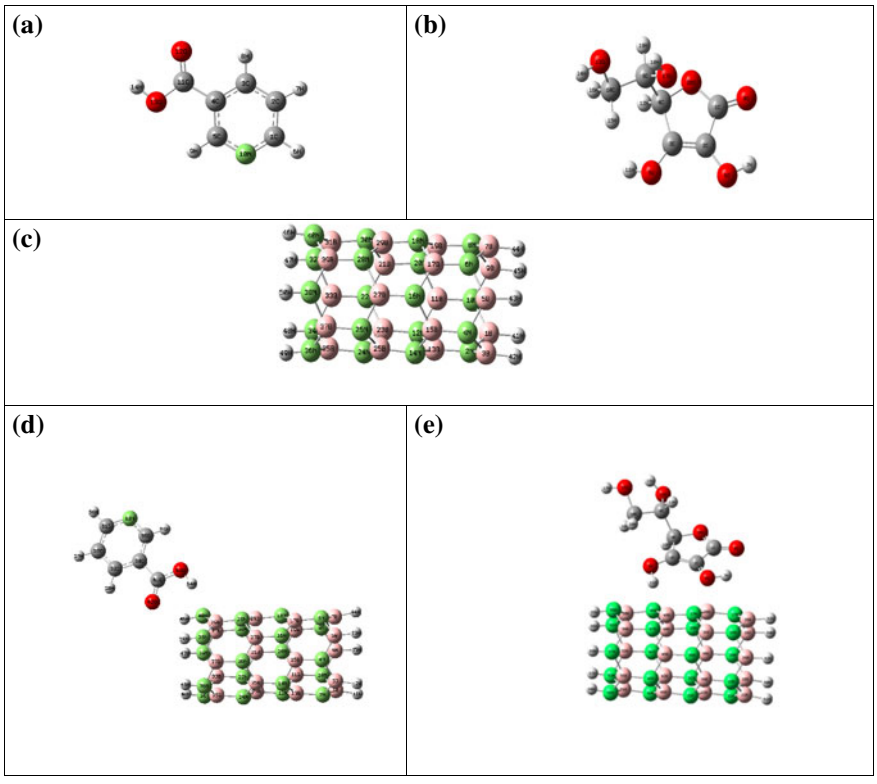

Figure 1. Fully optimized structures of (**a**) vitamin B3, (**b**) vitamin C, (**c**) (5, 0) BNNT, (**d**) BNNT-vitamin B3 complex and (**e**) BNNT-vitamin C complex.

the adsorption interaction. This indicates that BNNT prefers to adsorb vitamin B3 via the polar interaction rather than the π–π stack between the tube and the vitamin. As indicated by geometry of panel 'e' in figure 1, the furan ring in vitamin C slightly slopes to the tube surface, implying that there is π–π attraction interaction between the tube and vitamin C. Furthermore, the H atom in vitamin C also has polar interaction with N atom in the tube, as indicated by the calculated smallest N–H distance (table 1).[48]

To evaluate noncovalent adsorption between vitamins B3 and C and (5, 0) BNNT, we used the adsorption energy (E_{ad}), charge transfer (Q) and the equilibrium distance (D) between the (5, 0) BNNT and vitamin (equilibrium distance is defined as the nearest distance between atoms of respective vitamin and BNNT) (see table 1).

Table 1. Calculated E_{ad}(in eV), E_g(in eV), equilibrium distance, D(Å) and transferred charge (in e) of the BNNT-vitamin B3 and BNNT-vitamin C complexes.

System	E_{ad}(eV)	E_g(eV)	D(Å)	Q(e)
BNNT-vitamin B3	−0.530	4.013	1.883	−0.020
BNNT-vitamin C	−1.358	2.473	1.576	0.657

Adsorption energies of vitamin molecules on (5, 0) BNNT are calculated using the basis set superposition error (BSSE). This correction is done through the counterpoise method using ghost atoms as follows:

$$E_{ad} = E(\text{BNNT} - \text{vitamin}) - \left[E(\text{BNNT} - \text{vitamin}_{ghost}) + E(\text{vitamin} - \text{BNNT}_{ghost})\right], \quad (1)$$

where E (BNNT–vitamin) is the total energy of BNNT–vitamin complex. Ghost subsystems correspond to the additional localized basis centred at the atomic position of the vitamin or BNNT, but without any atomic potential. By including these ghost subsystems, correct binding energy is defined as the density functional theory total energy difference between the complex system and two subsystems.[49] $E_{ad} < 0$ denotes exothermic adsorption which means that the adsorption is stable energetically relative to the separated nanotube and vitamin. Results in table 1 show that absorption of vitamins B3 and C on (5, 0) BNNT is an exothermic process with adsorption energies of −0.530 eV and −1.358 eV, respectively. There is no chemical bond formation between the BNNT and vitamins B3 and C. Binding energy confirms that absorption process of vitamin B3 on BNNT is physisorption. In contrast, when vitamin C interacts with BNNT, absorption process is chemisorption.

On the other hand, influence of vitamins B3 and C adsorption on electronic properties such as spatial distribution of molecular orbitals (MOs), density of state (DOS), molecular orbital and charge transfer are important to obtain more details about the interaction of vitamins and BNNT.

Charge transfer is one of the key factors that facilities adsorption of adsorbate on the adsorbent. We provide the Q of vitamin molecules to BNNT using NBO[50,51] charges, which is less sensitive to the selected basis sets than the Mullikan[52] charge analysis. Noncovalent adsorption of vitamins B3 and C on the BNNT leads to an amount of charge transfer. The positive and negative values correspond to charge transfer from vitamin to (5, 0) BNNT and charge transfer from (5, 0) BNNT to vitamin, respectively. From table 1, it can be seen that charge transfer is −0.020 and 0.657 electrons for BNNT–vitamin B3 and BNNT–vitamin C complexes, respectively. Study of the adsorption energy and charge transfer of BNNT–vitamin B3 highlights that vitamin B3 and BNNT interact rather weakly, which is a result of the van der Waals attraction. Equilibrium distances (D) of (5, 0) BNNT and vitamins B3 and C are 1.883 Å ($R_{N40-H64}$) and 1.575 Å ($R_{N49-H12}$), respectively.

Energy levels of molecular orbitals, especially HOMO and LUMO, are excellent indicators of many molecular properties. We study the difference between HOMO and LUMO, known as the HOMO–LUMO energy gap ($E_g = E_{LUMO} - E_{HOMO}$). Calculated values of E_g of BNNT–vitamin B3 and BNNT–vitamin C complexes are given in table 1. The HOMO–LUMO energy gap of pure (5, 0) BNNT is 3.933 eV. Upon adsorption of vitamins B3 and C on tube, E_g of BNNT–vitamin B3 and BNNT–vitamin C complexes change to 4.013 and 2.473 eV, respectively. These results show that vitamin B3 absorption can little change electrical conductivity and transport properties of BNNT. Therefore, it can be concluded that BNNT cannot be an appropriate sensor for vitamin B3.

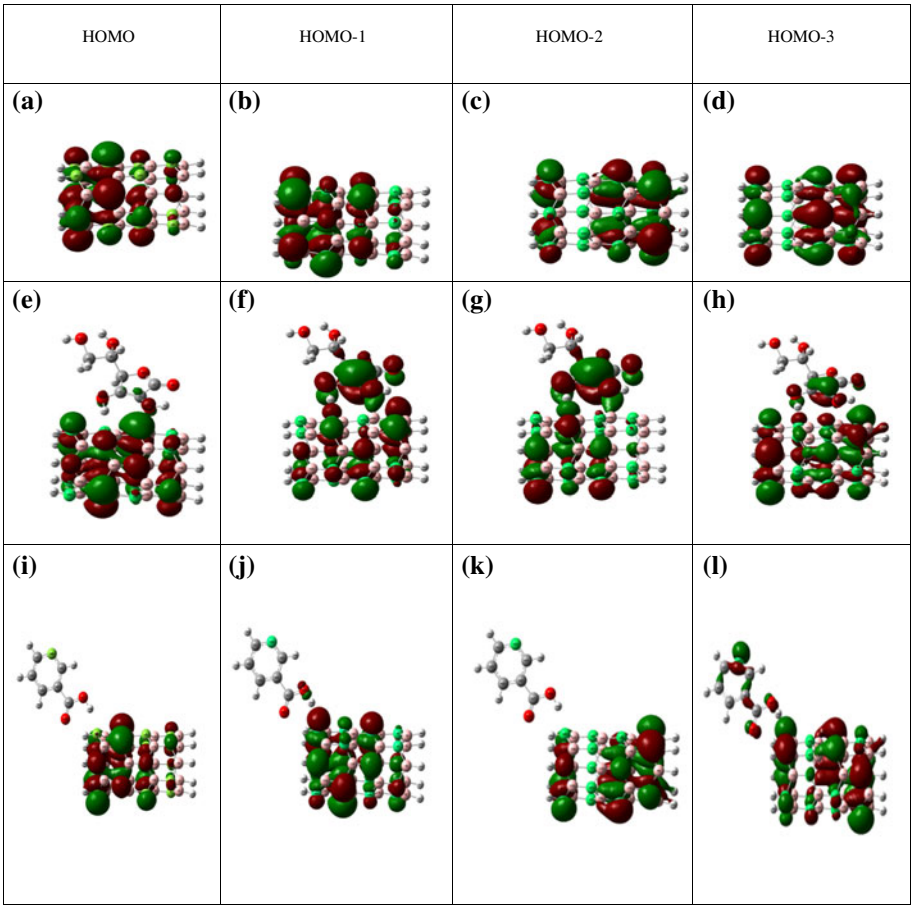

Figure 2. Orbital spatial distribution of HOMO, HOMO-1, HOMO-2 and HOMO-3 (**a**, **b**, **c**, **d**) optimized structure of (5, 0) BNNT (**e**, **f**, **g**, **h**) BNNT-vitamin C complex and (**i**, **j**, **k**, **l**) BNNT-vitamin B3 complex, respectively.

One of the important applications of noncovalent and covalent adsorption on BNNTs is to modify the electronic structures and thus widen their potential applications. The change in electro-conductivity of the BNNT systems is an important process in the sensor industry. It is well-known that E_g is a major factor determining the electrical conductivity of a material and there is a classic relation between them as follows:[53]

$$\sigma \propto \exp(-E_g/2kT), \tag{2}$$

where σ is the electrical conductivity, T is the temperature and k is the Boltzmann constant. According to the equation, larger E_g, at a given temperature, leads to smaller electrical conductivity. Therefore, the observed decrement in E_g of the BNNT upon the adsorption process leads to change in electrical conductivity of BNNT. In BNNT–vitamin C, E_g decreases from 3.933 for pristine BNNT to 2.473 eV upon adsorption of vitamin C. Considerable change in E_g value demonstrates high sensitivity of electronic properties of BNNT towards presence of vitamin C. Therefore, presence of vitamin C may be detected by calculating conductivity change of BNNT before and after the adsorption process. Results suggest that BNNT may be a promising candidate for serving as effective sensors to detect vitamin C.

It is worth mentioning that very strong interactions are not favourable in sensors because it implies that desorption of the adsorbate could be difficult and the device may suffer from long recovery times. If E_{ad} is significantly increased, much longer recovery time is expected based on the conventional transition state theory:

$$\tau = \exp \nu_0^{-1}(-E_{ad}/kT), \tag{3}$$

where T is the temperature, k is the Boltzmann constant, and ν_0 is the attempt frequency. According to this equation, more negative E_{ad} values will prolong recovery time in an exponential manner. Adsorption energy of vitamin C on BNNT is not too large to hinder recovery of BNNT and therefore the sensor will possess short recovery times.[54]

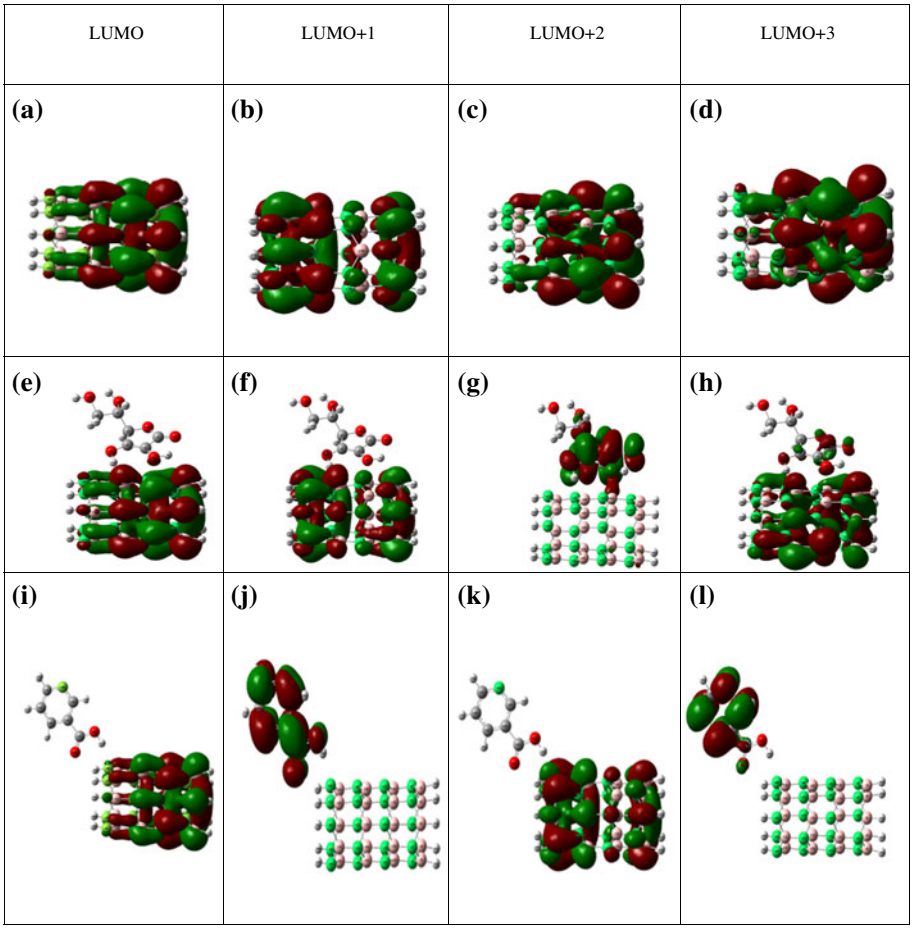

Figure 3. Orbital spatial distribution of LUMO, LUMO+1, LUMO+2 and LUMO+3 (**a**, **b**, **c**, **d**), optimized structure of (5, 0) BNNT (**e**, **f**, **g**, **h**), BNNT-vitamin C complex (**i**, **j**, **k**, **l**) and BNNT-vitamin B3 complex, respectively.

To further explain the electrical properties of BNNT–vitamin C and BNNT–vitamin B3 complexes and to examine the sensitivity of BNNT to vitamins, we studied spatial distribution of molecular orbitals including HOMO, HOMO-1, HOMO-2, HOMO-3 and LUMO, LUMO+1, LUMO+2, LUMO+3 and DOS. Spatial distribution was performed to obtain a better understanding of the interaction of vitamins C and B3 with (5, 0) BNNT. Figures 2 and 3 illustrate spatial distribution of HOMO, HOMO-1, HOMO-2, HOMO-3 and LUMO, LUMO+1, LUMO+2, LUMO+3 of the (5, 0) BNNT and BNNT–vitamin C and BNNT–vitamin B3 complexes. As shown in figure 2, HOMO and HOMO-1 of the (5, 0) zigzag BNNT model are located on the nitrogen atoms and mainly at the end of N-terminated and HOMO-2, and HOMO-3 is mainly distributed on the nitrogen atoms at the two ends of the tube and corresponds to the lone pair of electron on nitrogen atoms. In contrast, the LUMO, LUMO+2 and LUMO+3 are uniformly distributed throughout the B–N bonds and mainly at the ends of B-terminated and LUMO+1 is localized throughout the B–N bonds mostly at the two ends of the tube. The greatest extension values of LUMO suggest the high reactivity of the B–N pairs at the end of B-terminated towards nucleophilic attack. The small contribution of LUMO at N-terminated signifies less reactivity of these atoms towards nucleophilic attack. Figure 1b shows the highest contributions of electron density on nitrogen atoms and mainly at the end of N-terminated on the HOMO. This observation reveals that N-terminated is a highly favourable site for electrophilic attack.

For the (5, 0) BNNT–vitamin C, HOMO and HOMO-3 are mainly gathered on the nitrogen atoms of the

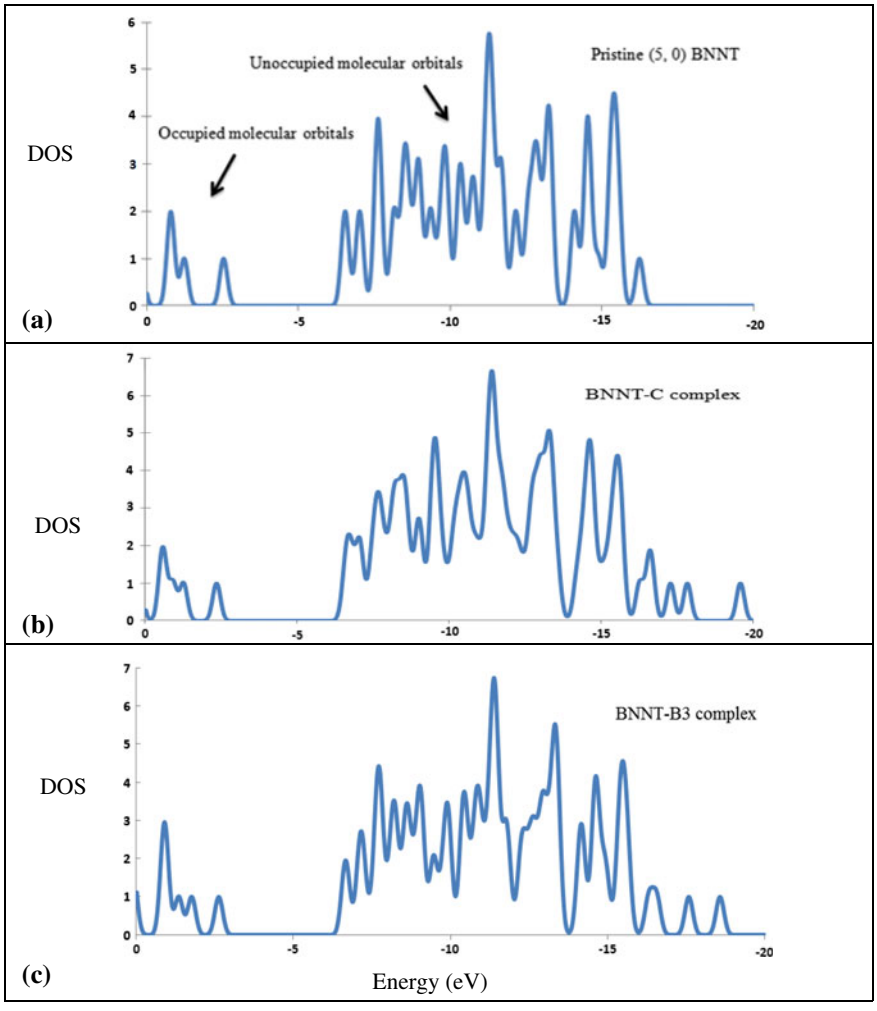

Figure 4. Density of states (DOS) of (**a**) pristine (5, 0) BNNT and noncovalent adsorption of (**b**) BNNT-vitamin C complex and (**c**) BNNT-vitamin B3 complex.

Table 2. Calculated E_{ad}(in eV), E_g(in eV), equilibrium distance, D(Å) and transferred charge (in e) of BNNT-radical vitamin B3 and BNNT-radical vitamin C on B and N sites.

System	E_{ad}(eV)	E_g(eV)	D(Å)	Q(e)
BNNT-radical vitamin B3 (B and N sites)	−1.010	3.628	1.515	−0.320
BNNT-radical vitamin C (B site)	−2.664	2.275	1.473	−0.223
BNNT-radical vitamin C (N site)	−1.063	2.024	1.456	−0.260

nanotube and HOMO-1, HOMO-2 are localized on the vitamin C ring and tube, while LUMO, LUMO+1 and LUMO+3 are distributed on the edge B–N bonds of the nanotube, which are basically due to unequal charge distribution along the edge B–N bonds and LUMO+2 are localized on the vitamin C ring.

Also figures 2 and 3 show that HOMO, HOMO-1, HOMO-2, HOMO-3 for the (5, 0) BNNT–vitamin B3 complexes are localized on the more electronegative nitrogen atoms, and LUMO and LUMO+2 of the BNNT–vitamin B3 complexes are distributed on the edge B–N bonds of the nanotube and LUMO+1

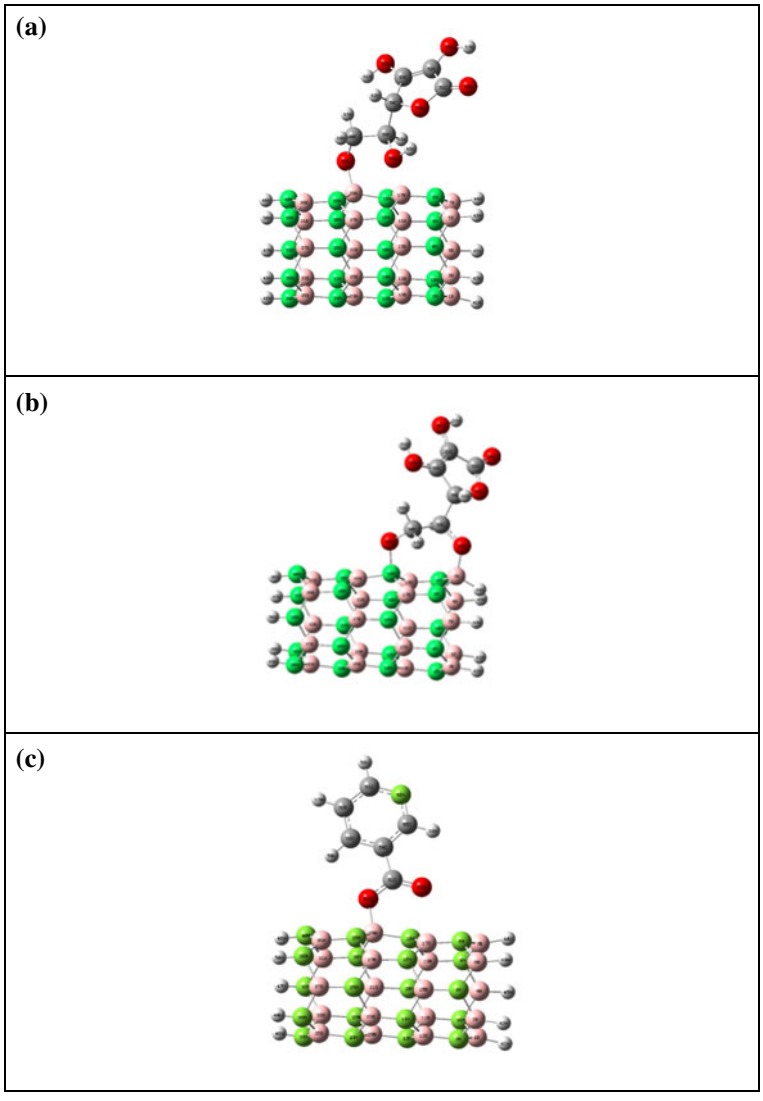

Figure 5. Fully optimized structures of (**a**) BNNT-radical vitamin C on B site, (**b**) BNNT-radical vitamin C on N site, (**c**) BNNT-radical vitamin B3 on B and N sites.

and LUMO+3 are localized on the vitamin B3 ring.

We calculated DOS of BNNT–vitamin C and BNNT–vitamin B3 complexes and compared with the pristine (5, 0) BNNT in figure 4. The DOS of the (5, 0) BNNT shows the significant changes due to vitamin C adsorption. The DOS plot of the BNNT–vitamin B3 shows that vitamin B3 noncovalent adsorption has no sensible effect on the electronic properties of BNNT; thus, in the noncovalent interaction of BNNT with vitamin B3, BNNT retains its original properties. On the other hand, from the energy point of view, vitamin B3 easily separate from the BNNT surface. Thus, we believe that the present result will provide useful guidance to develop novel BNNT-based drug delivery for vitamin B3.

3.2 *Covalent interaction of vitamins B3 and C with (5, 0) BNNT*

In this section, we report the interaction of vitamin B3 and C radicals with pristine (5, 0) BNNT. For covalent adsorption of vitamins B3 and C, one hydrogen atom was removed from hydroxyl group, and the remaining oxygen atom was brought closer to the B atom (B site) and N atom (N site) in the middle of the BNNT surface. Corresponding configurations were labelled BNNT-radical vitamin C and BNNT-radical vitamin B3. Optimized conformers are visualized in figure 5. Optimization geometries show that in the radical vitamin B3 at N site, a configuration similar to B site is formed. Also covalent interaction of radical vitamin C on N site leads to formation of a single covalent B_{7BNNT}-O_{64} bond.

Adsorption energies, charge transfer, band gap and equilibrium distance are presented in table 2. Equilibrium distance and calculated adsorption energies are found to be 1.515 Å and −1.010 eV for BNNT-radical vitamin B3 at B and N sites, 1.473 Å and −2.664 eV for BNNT–radical vitamin C at B site and 1.456 Å and −1.063 eV for BNNT–radical vitamin C at N site. Based on the calculated medium E_{ad} values, which indicate interaction between the tube and vitamins B3 and C radical is in a suitable extent (neither too weak to capture the molecule or too strong to be de-adsorbed), we consider BNNT could be used as potential adsorbents of vitamins B3 and C radical. Table 2 shows

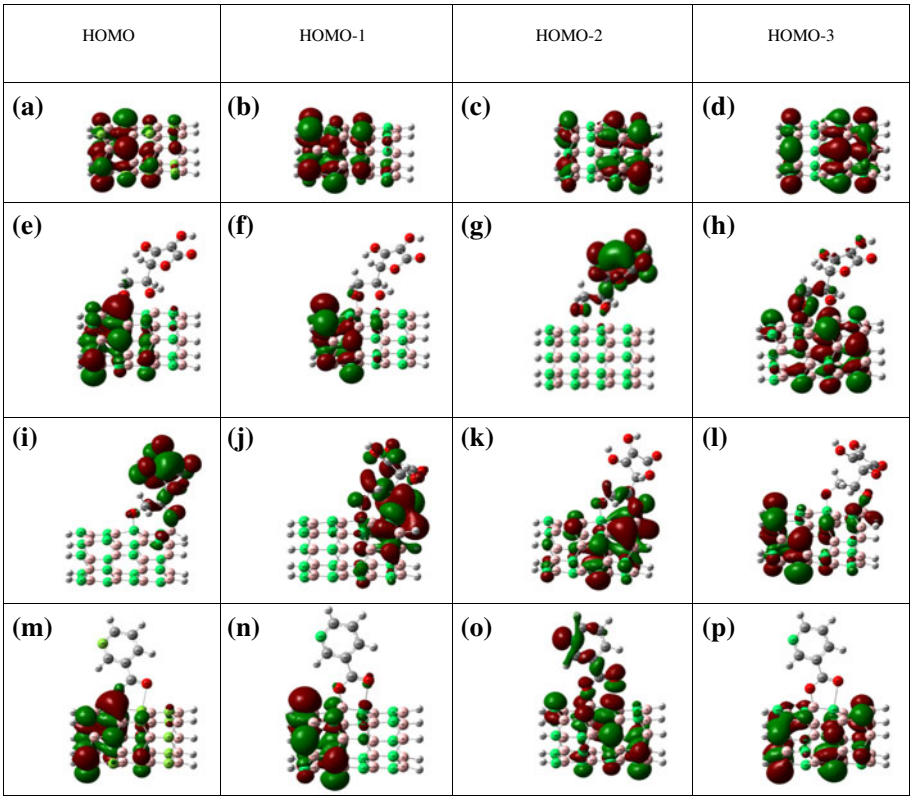

Figure 6. Orbital spatial distribution of HOMO, HOMO-1, HOMO-2 and HOMO-3 (**a**, **b**, **c**, **d**), optimized structure of (5, 0) BNNT (**e**, **f**, **g**, **h**), BNNT-radical vitamin C on B site (**i**, **j**, **k**, **l**) and BNNT-radical vitamin C on N site (**m**, **n**, **o**, **p**) and BNNT-radical vitamin B3 on B and N sites, respectively.

that transferred charge for all the systems is significant. Negative values of transferred charge for BNNT–radical vitamin B3 and BNNT–radical vitamin C at B and N sites correspond to the charge transfer from (5, 0) BNNT to vitamin.

In BNNT–radical vitamin B3, E_g decreases from 3.933 for pristine BNNT to 3.628 eV upon the adsorption of radical vitamin B3, indicating that the effect of adsorption process of vitamin B3 radical on BNNT conductance is negligible. This suitable interaction provides a potential way to functionalize BNNT without changing its electronic structure by vitamin B3 radical. Calculated E_g values of BNNT–radical vitamin C at B and N sites are 2.275 and 2.024 eV, respectively. Therefore, in comparison with the pristine BNNT (3.933 eV), adsorption of radical vitamin C at B and N sites on BNNT decreases energy gap of the tube, and increases their electrical conductance.

To get better insight into covalent interactions of BNNT with vitamin radicals, figures 6 and 7 show spatial distribution of molecular orbitals including HOMO, HOMO-1, HOMO-2, HOMO-3 and LUMO, LUMO+1, LUMO+2, LUMO+3. In the BNNT–radical vitamin C at B site (figure 6), HOMO and HOMO-1 are gathered on the nitrogen atoms of the nanotube and mainly at the end of N-terminated, HOMO-2 is mainly localized on the radical vitamin C and HOMO-3 is mainly gathered on the BNNT and vitamin. It can be seen from figure 7 that charge of LUMO is mostly distributed at the B-terminated of BNNT and LUMO+1 is gathered on the radical vitamin C, LUMO+2 and LUMO+3 are distributed mostly on the B–N bonds of the nanotube.

Also, it can be seen in figures 6 and 7 that in BNNT-radical vitamin C at N site, HOMO is localized over the radical vitamin C, HOMO-1 is gathered over the nanotube and radical vitamin C; whereas HOMO-2 and HOMO-3 are distributed on the (5,0) BNNT. The LUMO and LUMO+1 of the BNNT-radical vitamin C at N site are localized over the nanotube and the radical vitamin C and LUMO+2 and LUMO+3 are localized over the (5,0) BNNT.

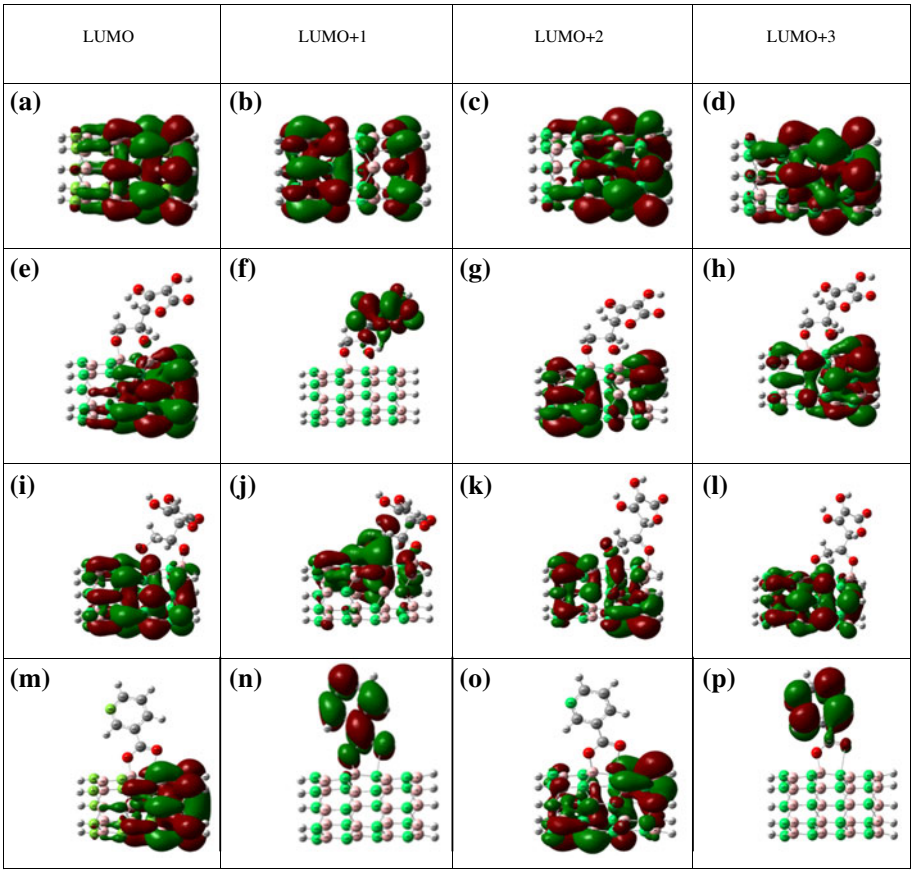

Figure 7. Orbital spatial distribution of LUMO, LUMO+1, LUMO+2 and LUMO+3 (**a**, **b**, **c**, **d**), optimized structure of (5, 0) BNNT (**e**, **f**, **g**, **h**), BNNT-radical vitamin C on B site (**i**, **j**, **k**, **l**) and BNNT-radical vitamin C on N site (**m**, **n**, **o**, **p**) and BNNT-radical vitamin B3 on B and N sites, respectively.

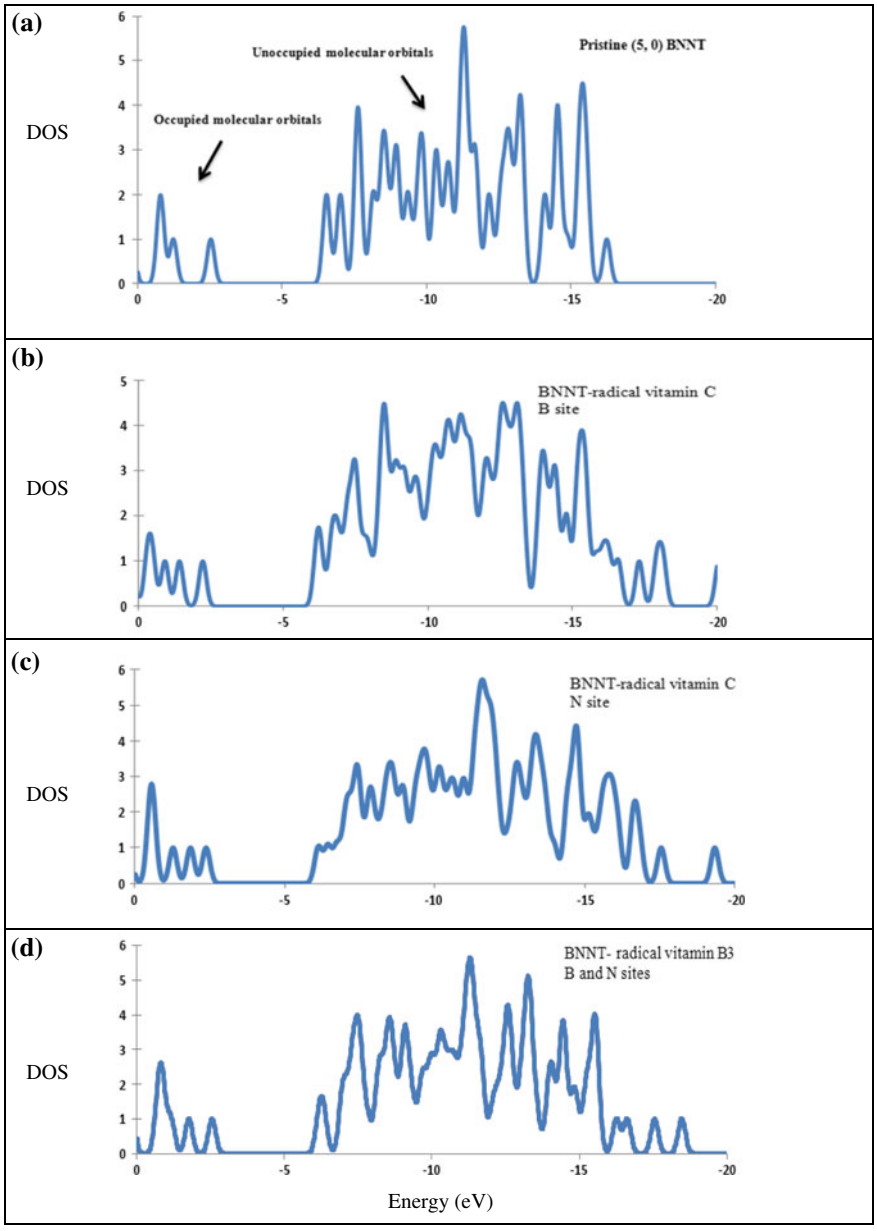

Figure 8. Density of states (DOS) of (**a**) pristine (5, 0) BNNT, (**b**) BNNT-radical vitamin C on B site, (**c**) BNNT-radical vitamin C on N site and (**d**) BNNT-radical vitamin B3 on B and N sites.

In BNNT-radical vitamin B3, HOMOs spread over the (5, 0) BNNT and LUMO and LUMO+2 are mostly localized on the nanotube, whereas LUMO+1 and LUMO+3 are distributed over the radical vitamin B3.

DOSs of pristine (5, 0) BNNT with adsorbed vitamins B3 and C radical are shown in figure 8. Compared with DOSs of the isolated BNNT, BNNT-radical vitamin C at B and N sites show remarkable changes due to vitamin C radical adsorption. This fact indicates that the (5, 0) BNNT presents a considerable change in the electronic and transport properties upon absorption of vitamin C radical at B and N sites. This result reveals a promising alternative for the use of BNNT as a sensing device to detect the vitamin C radical. It can be found in figure 8 that the DOS of BNNT-radical vitamin B3, is not affected by the radical vitamin B3 adsorption.

4. Conclusion

By performing density functional theory calculations, we have studied the noncovalent and covalent adsorptions of vitamins B3 and C on (5, 0) BNNT. We find

that the electronic properties of BNNT by the noncovalent and covalent interactions with vitamin B3 are little changed. These adsorptions are interesting because the vitamin can be easily removed from the BNNT surface, keeping original properties of the BNNT intact, which is one of the important factors for drug delivery. Hence, based on these theoretical results, BNNT can be used as material for delivery of vitamin B3.

Also, our calculations show that adsorption of vitamin C and vitamin C radical on BNNT is favourable from the energy point of view. We consider BNNT could be used as potential adsorbent of vitamins B3 radical. Electronic structures of BNNT present remarkable changes in the adsorption of vitamin C and its radical. Based on this theoretical result, we propose that BNNT can be used as a potential resource for vitamin C and vitamin C radical sensors. However, this study might be helpful in widening the application of BNNT in biosensors and drug delivery.

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