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Boron Nitride Nanotubes for Curcumin Delivery as an Anticancer Drug: A DFT Investigation

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Abstract: The electrical properties and characteristics of the armchair boron nitride nanotube (BNNT) that interacts with the curcumin molecule as an anticancer drug were studied using ab initio calculations based on density functional theory (DFT). In this study, a (5,5) armchair BNNT was employed, and two different interactions were investigated, including the interaction of the curcumin molecule with the outer and inner surfaces of the BNNT. The adsorption of curcumin molecules on the investigated BNNT inside the surface is a more favorable process than adsorption on the outside surface, and the more persistent and stronger connection correlates with curcumin molecule adsorption in this case. Furthermore, analysis of the HOMO–LUMO gap after the adsorption process showed that the HOMO value increased marginally while the LUMO value decreased dramatically in the curcumin-BNNT complexes. As a result, the energy gaps between HOMO and LUMO (Eg) are narrowed, emphasizing the stronger intermolecular bonds. As a result, BNNTs can be employed as a drug carrier in biological systems to transport curcumin, an anticancer medication, and thereby improve its bioavailability.

Keywords: DFT; boron nitride nanotube; armchair; curcumin; adsorption; HOMO–LUMO analysis; bioavailability

1. Introduction

Non-carbon nanostructures, as well as BNNTs, have attracted a lot of attention due to their thermal and chemical stability, together with their mechanical properties [1]. Boron nitride nanotubes (BNNTs) were originally introduced in 1994 [2], and the arc discharge procedure was used to produce them a year later [3]. Applications in various fields are extremely relevant for sensing applications [4], hydrogen storage [5], capture neutron therapy [6], drug delivery [7], and biomaterial applications [8]. Due to the theory of the adsorption of different molecules such as urea [9], CO2 [10], NH3 [11], Ni [12], and anticancer drugs [13] in nanotubes, various experiments have occurred in recent years.

For several years, one of the most significant nanomaterials studied in the pharmaceutical drug system has been carbon nanotubes (CNT) [14]. As CNTs are used as drug carriers, many biochemical problems arise concerning the interactions between drug molecules and carbon nanotubes. Experimentally and theoretically [15], there are many studies on this subject. One of the key challenges of nanocarriers is to encapsulate and release the drug in a nanoparticulate form without any chemical modifications at the proper site [16]. BNNT is a high inner volume nanocarrier that encapsulates more drugs and allows them to penetrate open ends [17]. The BNNTs are non-cytotoxic compared to carbon nanotubes (CNTs), with their large bandgap and the independence of electronic properties from the nanotube diameter, which is very chemically stable [18]. Curcumin is a tautomeric compound present in organic solvents as an enolic form and water as a keto form [19].
In history, curcumin was used as a medicinal herb for its different purposes, including antioxidant [20], anti-inflammatory [21], anti-mutagenic [22], anti-microbial [23], and other therapeutic attributes [24]. Curcumin is distributed as capsules, tablets, and ointments in many forms [25]. The U.S. Food and Drug Administration has accredited curcuminoids as “generally recognized as safe” (FDA) (GRAS) [26].

Curcumin is poorly absorbed and easily metabolized [27]. Functionalized single-walled carbon nanotubes (SWCNTs) have been used as a delivery system for curcumin molecules experimentally by Li et al. to protect curcumin from degradation and to increase its solubility [28]. They concluded that SWCNTs significantly enhance the solubility and stability of curcumin. To increase bioavailability, several agents were added. The most interesting is piperine; it increases curcumin bioavailability by blocking the metabolic pathway [29]. The goal of this paper is to investigate the adsorption of curcumin drugs on the inside and outside surfaces of armchair (5,5) BNNTs using density functional theory (DFT) calculations. As seen in Table 1, the details of the BNNT configuration (5,5) employed in this study together with the model in Figure 1, are shown.

**Table 1.** Properties of pristine BNNT.

| BNNT Configuration | Diameter (nm) | Bandgap (eV) |
|--------------------|---------------|--------------|
| (5,5)              | 9.872         | 4.71         |

2. Materials and Methods

2.1. Model System

The BNNT configuration (5,5) was chosen for this work because it has the highest stability following anticancer drug adsorption when compared to other BNNT configurations [30].

Using Virtual Nano Lab software (VNL 2017.1) [31], a total of two (2) identical BNNTs were created for the configuration after which the curcumin drugs interacted with the BNNTs via internal and external adsorption, resulting in two (2) different configurations of the BNNT-curcumin drug model. Adsorption was performed with no replacement of the boron or nitrogen atoms. These are illustrated in Figure 1.

2.2. Computational Details

The Quantum Espresso kit [31] was used to perform first-principal computations based on DFT/LDA. Plane-wave pseudopotentials in combination with LDA as functional exchange correlations, Ultrasoft pseudopotentials (XC), were used to simulate all electrons. The pseudopotential data set (Ultrasoft) utilized (H.pbe-nd-rrkjus psl.0.1), N. pz-n-rrkjus psl.0.1, O. pz-n-rrkjus psl.0.1, C. pz-n-rrkjus psl.0.1, and B. pz-n-rrkjus psl.0.1, pseudopotentials are given in Table 2 with electronic configurations. A plane-wave energy cut-off of 150 Rydberg was used. The Brillouin zone was sampled with $1 \times 1 \times 8$ special k-points for self-consistent field calculations using the Monkhorst Pack Scheme [32], and with $2 \times 2 \times 16$ for non-self-consistent field calculations (NSCF).

**Table 2.** Configurations of Pseudopotentials used in this work.

| Element | Pseudopotential Configuration | Valence Configuration |
|---------|-------------------------------|-----------------------|
| N       | $[\text{He}] 2s^2 2p^3 3d$    | $2s^1 2p^2$           |
| B       | $1s^2 2s^2 2p^1 3d^2$         | $2s^1 2p^2$           |
| C       | $[\text{He}] 2s^2 2p^2 3d^2$  | $2s^1 2p^2$           |
| O       | $[\text{He}] 2s^2 2p^4 3d^2$  | $2s^1 p^2$            |
| H       | $1s^1 2p^1$                  | $1s^1$                |
2.3. Loading Efficiency of Curcumin Molecules

In comparison to carbon nanotubes, the curcumin loading efficiency of BNNTs has been reported to be as high as 98.0 percent [28]. The large surface areas of BNNTs and curcumin’s molecular structure, which comprises two benzene rings and a conjugated ethylenic bond, both contribute to the high loading efficiency. Furthermore, because curcumin and BNNTs are both hydrophobic, the van der Waals forces between them will favor curcumin loading.

3. Results and Discussion

Figure 1 shows the optimized and interacting BNNT structures (5,5) with the curcumin medication inside and outside. The simulations were the band structure, density of states (DOS), and projected density of states (PDOS). The average bond length of B–N bonds after configuration optimization was 1.44, which is consistent with similar theoretical estimations for BNNTs [33]. Figure 2 shows the pure BNNT data, with Figure 2a showing the band structure for (5,5) BNNT. The wider bandgap calculated in this figure indicates that the BNNT is insulating. This is further supported by the DOS result in Figure 2b, which shows a large bandgap separating the high densities of states seen in the valence band from the relatively low levels seen in the conduction band. The BNNT’s calculated band gap is 4.71. This bandgap, which may be attributed to the underestimation of the DFT bandgap [34], is smaller than other theoretically measured band gaps between 5.0 and 6.0 eV [35].

Figure 1. The optimized structure of (a) (5,5) BNNT, (b) curcumin drugs and their adsorption, (c) inside and (d) outside the BNNT.
3.1. Molecular Geometry and Adsorption Energy

Curcumin molecules on the outer and inner surfaces of the BNNTs used as drug carriers were geometrically optimized to achieve the most stable configuration. After geometric optimization, the stable configuration is obtained. Figure 1 shows the optimal geometry of curcumin, BNNTs, and curcumin-BNNT complexes. As can be seen in Table 3, the optimized diameter for (5,5) BNNT is 7.191. This value is acceptable and comparable to previously reported values [36].

Table 3. The simulated system.

| System          | BNNT Type | Drug Position | Number of Atoms |
|-----------------|-----------|---------------|-----------------|
| Curcumin-(5,5)  | (5,5)     | outside       | 50              |
| BNNT            | 7.191     |               | 50              |
| Curcumin-(5,5)  | (5,5)     | inside        | 50              |
| BNNT            | 7.191     |               | 50              |

Table 4 shows the determined adsorption values of HUMO, LUMO energies, and energy gap (Eg). As can be seen in Table 4, the calculated adsorbing energy value was 15.15 Kcal/mol, at the level of the LDA + DFT theory, for the adsorbed curcumin on the outer surface of (5,5) BNNT. The system analysis showed that the adsorption energy value is negative. Thus, the drug and the nanotube interact more favorably. As a consequence, the adsorption of curcumin drugs on the external surface of the nanotube is beneficial and exothermic. This finding allows for the physical adsorption of the curcumin molecule on the external surface of the nanotube studied. The adsorbent energy value is 16.91 kcal/mol at levels of LDA + DFT theory for the adsorbed curcumin molecule within the (5,5) nanotube. Our finding indicates the perfect adsorption of curcumin molecules inside the (5,5) nanotube.
nanotube, and the highest energy absorbance value has been increased for the molecule inside the studied nanotube. In the reported results of Table 4, the higher adsorption energy (E_{ads} = 16.91 \text{ kcal/mol}) corresponds to the adsorption of the curcumin molecule inside of the (5,5) nanotube.

Table 4. The adsorption energies and the geometric parameters of curcumin drug adsorbed on the BNNTs.

| System          | Position | E_{ads} (kcal/mol) | EHOMO (eV) | ELUMO (eV) | Eg (eV) |
|-----------------|----------|--------------------|------------|------------|---------|
| Curcumin        |          | −5.03              | −1.22      | 3.81       |         |
| (5,5) BNNT      | outside  | −5.68              | −0.96      | 4.71       |         |
| Curcumin-(5,5) BNNT | outside | −15.15             | −4.84      | −1.22      | 3.62    |
| Curcumin-(5,5) BNNT | inside  | −16.91             | −4.94      | −1.29      | 3.65    |

3.2. Electronic Properties

In this section, we study the effect of the electronic properties of BNNT on curcumin adsorption. In Table 4, the calculated HOMO and the LUMO energies and energy gap (the difference between the HOMO and LUMO energies for the pristine curcumin molecule, BNNT, and the curcumin-BNNT complexes at the theoretical level of LDA + DFT) have been reported. The energy gap (E_{g}) is an important element in chemical reactivity determination and charge transfer. The energy gap was determined to track the stability of the complexes. Lower LUMO energy molecules are more likely to accept electrons and have higher electrophilicity. Electrons from molecules of higher LUMO energy values can be accepted by the molecules. Higher HOMO energy values contribute to nucleophilicity. The HOMO–LUMO energy band gap of a system is associated with a decrease or increase in chemical reactivity and chemical stability. Since the HOMO–LUMO energy gap (E_{g}) of the curcumin drug inside the BNNTs complex has an increase in the molecular energy gap, it is then associated with a decrease in chemical reactivity and an increase in stability. This means overcoming the barriers to adequate curcumin delivery, thus improving its bioavailability.

The value of the HOMO–LUMO energy gap (E_{g}) for pristine (5,5) BNNT was found to be 4.71 (Table 4). After the adsorption process of curcumin molecules on the (outside and inside) surfaces of (5,5) BNNT, E_{g} values were found to be 3.62 and 3.65 eV, respectively. For both complexes, HOMO and LUMO energies are adjusted to higher and lower energies, respectively, which results in a decrease in the E_{g} value of the complex (Table 4). The E_{g} of the adsorbed molecule on the inner surface of the (5,5) BNNT is higher than the E_{g} adsorbed molecule on the outer surface of the (5,5) BNNT. The drug molecule has better adsorption and more stability inside than outside for (5,5) BNNT. All these findings agree and accept the results of previous results seen in this review, so drug molecules are better adsorbed inside the (5,5) BNNT surface according to the adsorption energy (Table 4). Increased electrical conductivity of the complexes is predicted by the comparisons between the E_{g} of the drug molecule and the pristine BNNT of the complexes. Density of states (DOS) diagrams for curcumin drug, (5,5) BNNT, and curcumin drug complexes with (5,5) BNNT are shown in Figure 3. The energy level and peaks of the panel (c) are compared with those of panel (b) to show the adsorption of the nanotubes studied. As seen in Figure 3, a slight change is observed near the valence band after adsorption of drug molecules within (5,5) BNNT compared to that of the pristine (5,5) BNNT.
In our work, we studied the BNNT interactions between the armchair (5,5) BNNT and the curcumin molecule in both the inner and outer positions of the nanotube with the DFT method. The results show that the drug molecule studied can adsorb both in the outer and inner positions of (5,5) BNNT, but has better adsorption in the inner position. It has been observed that the HOMO values increased marginally after adsorption, while the LUMO value in these systems decreased considerably in the curcumin-BNNT structures, thus reducing the energy gap ($E_g$). This result further indicates an increase in the electrical conductivity of these systems. As a result, it was found that the curcumin drug can be physically adsorbed by the walls of the studied BNNT, and that the BNNT can reliably perform as a carrier for curcumin drug molecules in drug delivery to eventually improve the bioavailability of the drug studied.

**Figure 3.** DOS for a (5,5) BNNT-curcumin complex; (a) inside position, and (b) outside position.

### 4. Conclusions

In our work, we studied the BNNT interactions between the armchair (5,5) BNNT and the curcumin molecule in both the inner and outer positions of the nanotube with the DFT method. The results show that the drug molecule studied can adsorb both in the outer and inner positions of (5,5) BNNT, but has better adsorption in the inner position. It has been observed that the HOMO values increased marginally after adsorption, while the LUMO value in these systems decreased considerably in the curcumin-BNNT structures, thus reducing the energy gap ($E_g$). This result further indicates an increase in the electrical conductivity of these systems. As a result, it was found that the curcumin drug can be physically adsorbed by the walls of the studied BNNT, and that the BNNT can reliably perform as a carrier for curcumin drug molecules in drug delivery to eventually improve the bioavailability of the drug studied.

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References

1. Kostoglou, N.; Tampaxis, C.; Charalambopoulou, G.; Constantinides, G.; Ryzhkov, V.; Doumanidis, C.; Matovic, B.; Miterrer, C.; Rebholz, C. Boron nitride nanotubes versus carbon nanotubes: A thermal stability and oxidation behavior study. *Nanomaterials* **2020**, *10*, 2435. [CrossRef] [PubMed]

2. Alshammari, N. Joining between Boron Nitride Nanocones and Nanotubes. *Adv. Math. Phys.* **2020**, *2020*. [CrossRef]

3. Yanar, N.; Yang, E.; Park, H.; Son, M.; Choi, H. Boron nitride nanotube (BNNT) membranes for energy and environmental applications. *Membranes* **2020**, *10*, 430. [CrossRef] [PubMed]

4. Ding, H.; Guan, J.; Lu, P.; Mihailov, S.J.; Kingston, C.T.; Simard, B. Boron nitride nanotubes for optical fiber chemical sensing applications. *IEEE Sens. Lett.* **2020**, *4*, 1–4. [CrossRef]

5. Panigrahi, P.; Kumar, A.; Bae, H.; Lee, H.; Ahuja, R.; Hussain, T. Capacity enhancement of polythiatriated functionalized boron nitride nanotubes: An efficient hydrogen storage medium. *Phys. Chem. Chem. Phys.* **2020**, *22*, 15675–15682. [CrossRef] [PubMed]

6. Dymova, M.A.; Taskaev, S.Y.; Richter, V.A.; Kuligina, E.V. Boron neutron capture therapy: Current status and future perspectives. *Cancer Commun.* **2020**, *40*, 406–421. [CrossRef] [PubMed]

7. Khalili, N.P.; Moradi, R.; Kavehpour, P.; Islamzada, F. Boron nitride nanotube clusters and their hybrid nanofibers with polycaprolacton: Thermo-PH sensing drug delivery functional materials. *Eur. Polym. J.* **2020**, *127*, 109585. [CrossRef]

8. Lee, S.H.; Kim, M.J.; Ahn, S.; Koh, B. Purification of boron nitride nanotubes enhances biological application properties. *Int. J. Mol. Sci.* **2020**, *21*, 1529. [CrossRef]

9. Joy, J.; George, E.; Haritha, P.; Thomas, S.; Anas, S. An overview of boron nitride based polymer nanocomposites. *J. Polym. Sci.* **2020**, *55*, 3115–3141. [CrossRef]

10. Maurya, M.; Sappidi, P.K.; Singh, J.K. Selective Separation of CO2 from flue Gas Using Carbon and Boron Nitride Nanotubes as a Membrane. *Energy Fuels* **2020**, *34*, 7223–7231. [CrossRef]

11. Mohsennia, M.; Rakhsi, M.; Rasa, H. A computational study on interactions of Ni- and Pt-doped boron nitride nano tubes with NH3 in presence and absence of electric fields. *Comput. Theor. Chem.* **2018**, *1136*, 1–9. [CrossRef]

12. Marko, Š.; Snezana, M.; Marijana K., I.; Jasmina, N.; Malcolm, W.; Zoltan, K.; Jelena, T. Comparing the adsorption performance of multilayered carbon nanotubes oxidized by varying degrees for removal of low levels of copper, nickel and chromium(VI) from aqueous solutions. *Water 2020*, *12*, 723. [CrossRef]

13. Zarghami Dehaghani, M.; Yousefi, F.; Sajadi, S.M.; Tajammal Munir, M.; Abida, O.; Habibzadeh, S.; Mashhadzadeh, A.; Rabiee, N. Mostafavi, E.; Saeb, M.R. Theoretical encapsulation of fluorouracil (5-fu) anti-cancer chemotherapy drug into carbon nanotubes (cnt) and boron nitride nanotubes (bnnt). *Molecules* **2021**, *26*, 4920. [CrossRef]

14. Jha, R.; Singh, A.; Sharma, P.K.; Fuloria, N.K. Smart carbon nanotubes for drug delivery system: A comprehensive study. *J. Drug Deliv. Sci. Technol.* **2020**, *58*, 101811. [CrossRef]

15. Sohrabi, N.; Alighosseini, A.; Pirouzfar, V.; Pedram, M.Z. Analysis of dynamics targeting CNT-based drug delivery through lung cancer cells: Design, simulation, and computational approach. *Membranes* **2020**, *10*, 283. [CrossRef]

16. Pham, D.T.; Tiyaboonchai, W. Fibroin nanoparticles: A promising drug delivery system. *Drug Deliv.* **2020**, *27*, 431–448. [CrossRef] [PubMed]

17. Gahremanes, S.; Samadizadeh, M.; Khaleghian, M.; Shiraz, N.Z. Theoretical study of encapsulation of Fluoxuridine anticancer drug into BN (9,9-7) nanotube for medical application. *Phosphorus Sulfur Silicon Relat. Elem.* **2020**, *195*, 293–306. [CrossRef]

18. Genchi, G.G.; Rocca, A.; Grillone, A.; Marino, A.; Ciofani, G. Boron nitride nanotubes in nanomedicine: Historical and future perspectives. *In Boron Nitride Nanotubes in Nanomedicine*; Elsevier: Amsterdam, The Netherlands, 2016; pp. 201–217.

19. Rathore, S.; Mukim, M.; Sharma, P.; Devi, S.; Nagar, J.C.; Khalid, M. Curcumin: A Review for Health Benefits. *Int. J. Res. Rev.* **2020**, *7*, 273–290.

20. Reda, F.M.; El-Saadony, M.T.; Elnser, S.S.; Alagawany, M.; Tufarelli, V. Effect of dietary supplementation of biological curcumin nanoparticles on growth and carcass traits, antioxidant status, immunity and caecal microbiota of Japanese quails. *Animals* **2020**, *10*, 754. [CrossRef]

21. Manoharan, Y.; Haridas, V.; Vasanthakumar, K.C.; Muthu, S.; Thavoorullah, F.F.; Shetty, P. Curcumin: A Wonder Drug as a Preventive Measure for COVID-19 Management. *Indian J. Clin. Biochem.* **2020**, *35*, 373–375. [CrossRef]

22. Akram, M.; Riaz, M.; Vadood, A.W.C.; Hazrat, A.; Mukhtar, M.; Ahmad Zakki, S.; Daniyal, M.; Shariati, M.A.; Said Khan, F.; Zainab, R.; Sajjadi, M.; Sharifir, S.; Fathi, N.; Memar, M.Y.; Hosseinian Khatibi, S.M.; Khalilov, R.; Nezhad, R.; Negahdari, R.; Zunini Vahed, S.; Maleki Dizaj, S.; Moravej, H.; et al. Therapeutic effects of supplementation with Curcuminoids in critically ill patients receiving enteral nutrition: A randomized controlled trial protocol. *J. Diabetes Metab. Disord.* **2020**, *19*, 1609–1614. [CrossRef]

23. Bresciani, L.; Favari, C.; Calani, L.; Francinelli, V.; Riva, A.; Petrangolini, G.; Allegrini, P.; Mena, P.; Del Rio, D. The effect of formulation of curcuminoids on their metabolism by human colonic microbiota. *Molecules* **2020**, *25*, 940. [CrossRef] [PubMed]
28. Li, H.; Zhang, N.; Hao, Y.; Wang, Y.; Jia, S.; Zhang, H.; Zhang, Y.; Zhang, Z. Formulation of curcumin delivery with functionalized single-walled carbon nanotubes: Characteristics and anticancer effects in vitro. *Drug Deliv.* 2014, 21, 379–387. [CrossRef]

29. Chen, S.; Li, Q.; McClements, D.J.; Han, Y.; Dai, L.; Mao, L.; Gao, Y. Co-delivery of curcumin and piperine in zein-carrageenan core-shell nanoparticles: Formation, structure, stability and in vitro gastrointestinal digestion. *Food Hydrocoll.* 2020, 99, 105334. [CrossRef]

30. Hosseinzadeh, B.; Beni, A.S.; Eskandari, R.; Karami, M.; Khorram, M. Interaction of propylthiouracil, an anti-thyroid drug with boron nitride nanotube: A DFT study. *Adsorption* 2020, 26, 1385–1396. [CrossRef]

31. Sukhender; Pravesh, P.; Mohan, L.; Verma, A.S. First principles calculations for electronic, optical and magnetic properties of full heusler compounds. *East Eur. J. Phys.* 2020, 2020, 111–121. [CrossRef]

32. Giannozzi, P.; Baseggio, O.; Pietro, B.; Bruno, D.; Car, R.; Cavazzoni, C.; De Gironcoli, S.; Delugas, P.; Ferrari Ruffino, F. Quantum ESPRESSO toward the exascale. *J. Chem. Phys.* 2020, 152, 154105. [CrossRef] [PubMed]

33. Wasfi, A.; Awwad, F.; Ayesh, A.I. DNA sequencing via Z-shaped graphene nano ribbon field effect transistor decorated with nanoparticles using first-principle transport simulations. *New J. Phys.* 2020, 22, 063004. [CrossRef]

34. Legesse, M.; Rashkeev, S.N.; Saidou, H.; el Mellouhi, F.; Ahzi, S.; Alharbi, F.H. Band gap tuning in aluminum doped two-dimensional hexagonal boron nitride. *Mater. Chem. Phys.* 2020, 250, 123176. [CrossRef]

35. Shokri, A.; Yazdani, A.; Rahimi, K. Possible bandgap values of graphene-like ZnO in density functional theory corrected by the Hubbard U term and HSE hybrid functional. *Mater. Today Commun.* 2020, 22, 100756. [CrossRef]

36. Mojarrab, M.; Ashshadi, M. Tight-binding method for the electronic and optical properties of C and BN nanotubes. *Mater. Sci. Eng. B Solid-State Mater. Adv. Technol.* 2020, 261, 114671. [CrossRef]