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EXPLORING THE ADSORPTION POTENTIAL OF CARBON NANOTUBES AS EFFICIENT ADSORBERS FOR DRUG MOLECULES

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Abstract: This research observed the interaction between carbon nanotubes (CTs) and ephedrine (EH) molecules through a comprehensive utilization of density functional theory (DFT) and density functional tight-binding (DFTB) calculations applied to both periodic and isolated structures. EH, as a prevalent pharmaceutical pollutant, interacts with CTs and prominent organic nanostructures, prompting a meticulous examination of CTs' potential as EH adsorbents. Multiple models of CTs were systematically scrutinized to elucidate their interaction with EH in detail. Given the substantial complexity of systems involving 122-187 atoms, the DFTB methodology was used for geometric optimizations. DFT computations were subsequently employed to procure accurate total energies, enabling the precise evaluation of binding energies between EH and nanotubes. The binding energies, ranging from –0.46 eV to –0.53 eV, confirm significant non-covalent interactions between CTs and EH. The shortest distance between EH and CT in all observed systems involves the hydrogen atom in the vicinity of the oxygen atom which is also crucial for non-covalent interactions. The outcomes underscore the propensity of CTs to adsorb EH molecules with notable binding energies, striking a balance between robust adhesion and facilitation of desorption under plausible experimental conditions. These findings not only shed light on the fundamental mechanisms governing the CT-EH interaction but also offer promising insights for the practical application of CTs in environmental remediation strategies targeting pharmaceutical pollutants.

Keywords: Pharmaceuticals, DFT, binding energies, environmental remediation.

1. INTRODUCTION

Ephedrine (EH) is a crucial component of the ephedra plant, a traditional medicine known for its anti-asthmatic and antitussive properties [1]. This compound, derived from aromatic amino alcohols, possesses diverse biological activities as a significant alkaloid. Its primary pharmacological effects include vasoconstriction, elevation of blood pressure, bronchodilation, and stimulation of the central nervous system [2]. EH is utilized in the treatment of influenza, asthma, and hypotension, and it has also been exploited as a precursor for the illicit production of methamphetamine, a potent stimulant, through a straightforward chemical process [3]. Research findings reveal EH as a prevalent substance in 7 urban rivers in Beijing, reaching a maximum concentration of 185.7 ng/dm^3. The highest concentration of EH was recorded in the United States, where 6.9 mg/dm^3 was detected in the wastewater influents. In England, EH levels varied between 8.7 and 1979.5 ng/dm^3, while Spanish river water exhibited concentrations ranging from 0.7 to 145.0 ng/dm^3 [4]. The significant presence of EH in aqueous environments, coupled with its frequent detection, suggests widespread usage worldwide. Notably, as an emerging environmental contaminant, EH poses potential risks to ecosystems [5, 6].

Since various pharmaceuticals, such as EH, have been detected in waters, the scientific community is committed to finding new methods for their removal. Removal of pharmaceutics can be achieved in different ways; however, adsorption remains one of the most essential methods for extracting the selected pharmaceuticals and developing new devices to determine and quantify pharmaceuticals. For adsorption, organic nanomaterials have drawn the significant attention of scientists. In these regards, nanotubes, fullerenes, and graphene are considered materials with outstanding potential for practical applications in the adsorption of pollutants.

Carbon nanotubes (CT) have been particularly popular in water treatment due to their specific structure and outstanding adsorption properties [7, 8]. In addition to their supreme adsorption properties, these materials can be obtained using various methods, including arc discharge, laser ablation, and catalytic vapor deposition [9–11]. They are also readily available for modifications to achieve desired physical and chemical properties [12–14].

CTs have been studied as adsorbers of different materials in many experimental and theoretical studies. However, the adsorption by nanotubes is frequently modeled by considering the nanotube as a molecule whose ends are terminated with hydrogen molecules. Of course, this is a valid model, but only if the nanotube model is of significant length. Frequently, short models of hydrogen-terminated nanotubes are considered, so if the large pharmaceutical molecule is adsorbed, it actually interacts with hydrogen atoms with which the nanotube is terminated. These are not realistic models, as they do not take properly into account the periodicity of nanotubes.

Aside from the large “molecular” model of the nanotube, to properly investigate adsorption, DFT calculations on periodic structures are required, which is undoubtedly computationally demanding. In this study, a combination of DFT calculations on both periodic and molecular systems has been applied to understand the interactions between CTs and the EH molecule. With these results, we aim to estimate the potential of CTs to adsorb the EH molecule, which is essential for developing methods for the removal of EH from water.

2. COMPUTATIONAL DETAILS

Different quantum-mechanical theory levels have been applied to understand interactions between CTs and EH molecules. The density functional tight-binding (DFTB) method [15–18] on periodic systems containing carbon nanotube and EH has been utilized to perform geometrical optimizations. Slater-Koster files from the “matsci” library of parameters [19, 20] have been used for all DFTB calculations.

While all systems considered for the calculation of binding energies have been geometrically optimized at the DFTB level, total energies have been re-calculated at the DFT level to achieve better accuracy. A PBE [33] functional was used in the DFT calculations on periodic systems, together with a double zeta polarized basis set.

To obtain information about the intermolecular non-covalent interactions (NCI) between CTs and EH molecules, periodic systems have been transformed into molecular systems. After that, the DFT calculations on molecular systems have been performed using the B3LYP functional [21], together with the MIDIX basis set [22–24].

All DFTB and DFT calculations on periodic systems have been performed with QuantumATK 2015.3 modeling package [25–27], while DFT calculations on molecular systems have been performed with Jaguar [28,29] program, as implemented in Schrödinger Materials Science Suite 2021-1.

3. RESULTS AND DISCUSSION

3.1. Structural considerations

In this work, we have decided to study the adsorption of EH on three models of CTs described by the following chiral vectors: (6,0), (8,0), and (10,0). The smallest model considered in this work, the (6,0), is frequently employed in computational studies. Larger nanotube models (8,0) and (10,0), contain a significantly higher number of carbon atoms and may be computationally demanding. To generate the systems for DFT calculations, the EH molecule was placed above the CT in an orthorhombic unit cell, after which the geometrical optimizations were performed. The following naming of the systems has been adopted: CT:EH(n,0), where *n* denotes the value of the chiral vector, which in this work principally determines the size of the nanotube.

To study the adsorption of the EH molecule, it was necessary to repeat each model four times of each model in *z*-direction. Repetition of CTs together with the EH molecule placed above the nanotube led to the models that contained 123, 155, and 187 atoms for systems CT:EH(6,0), CT:EH(8,0) and CT:EH(10,0), respectively.

The very high number of atoms in each system induced the necessity of applying the DFTB level of theory for geometrical optimizations. This level of theory is known to produce reasonable geometries at a fraction of the time compared to the DFT level.

3.2. Binding energies

Binding energy is undoubtedly one of the most critical parameters principally regulating the adsorption properties of some materials. To bind some molecules, binding energy should have a high magnitude. On the other hand, the binding energy shouldn't be too high because desorption wouldn't be possible under reasonable experimental conditions, and it is not possible to re-use adsorber. If the binding energies are of adequate magnitudes, desorption might occur by simple heating.

For these reasons, it is imperative to achieve non-covalent binding between the adsorber and the adsorbed molecule. Binding energies up to 1 eV are related to NCI, and therefore, it is desirable to achieve binding with limits up to this range. Binding energies obtained in this work are summarized in Figure 1.

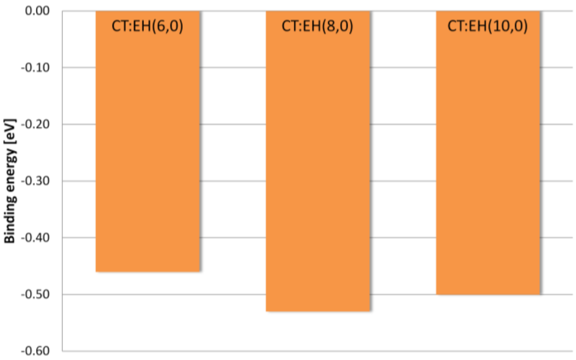

Figure 1. *Binding energies between selected nanotubes and EH.*

Results presented in Figure 1 indicate that strong binding occurs between considered CTs and EH molecules. Considering the binding energies, there is no particular trend with respect to the size of studied nanotubes. The binding energies have similar values ranging from –0.46 eV to –0.53 eV. The obtained results are significant and confirm that the non-covalent binding occurs between CTs and EH since the binding energies are lower than 1 eV.

In a Dai et al. [43] study, the adsorption properties of CTs towards the selected gaseous volatile organic compounds have been studied employing the DFT calculations. The binding energies obtained in this study ranged from –0.16 eV (for methane) to –0.63 eV (for toluene). Novir et al. [30] computationally investigated the adsorption of COVID-19-related drug remdesivir on pristine and modified CTs. When the B3LYP/3-21G level of theory was applied, they obtained binding energies between CT (5,5) and remdesivir to be in a range from –0.12 eV to –0.25 eV, depending on the configuration.

Boron-nitride nanotubes have also been frequently considered as adsorbers in various computational studies. For example, Chigo-Anota et al. [31] investigated the adsorption of paracetamol drug by (5,5) boron-nitride nanotube and obtained a binding energy equal to –0.48 eV. Adsorption of paracetamol by (5,5) boron-nitride nanotube was also a subject of the study performed by Ghasempour et al. [32], in which they obtained the binding energy to be –0.91 eV. They also investigated the adsorption of phenacene, for which they obtained a binding energy of –1.16 eV. All of the reports from similar studies clearly indicate that the binding energies obtained in this study are highly representative. Both conditions, relatively strong binding energies lower than 1 eV, have been obtained in the case of adsorption of EH by CTs, which was a motivation for further calculations.

3.3. Non-covalent interactions

To understand which parts of the EH molecule are principally responsible for the interactions with CTs, an analysis of electron density between all atoms has been performed. This was achieved by calculations on the basis of methods reported in references [33, 34], which are also incorporated in the Jaguar program. Additionally, π-π interactions on the basis of geometrical criteria have also been analyzed in this work to gain a deeper understanding of the calculated binding energies.

The strengths of intermolecular NCI, which formed between CTs and the EH molecule, have been illustrated in Figure 2. To run NCI calculations with the Jaguar program, the periodic system first had to be transformed into a molecular one. The positions of atoms were adopted from the crystal structure, but to adjust the structure for molecular DFT calculations, CTs were terminated with hydrogen atoms. To optimize terminal hydrogen atoms' positions, constrained DFTB calculations were run during which positions of all atoms but the terminal hydrogen atoms were fixed.

As indicated in Figure 2, EH forms five NCIs with CTs in all cases. In each case, the strongest NCI involved the hydrogen atom of EH circled in Figure 3. In this particular case, the strength of NCI is almost two times higher than any other NCI formed between EH and CT.

Considering the importance of the benzene ring in nanotubes, we were also interested in π-π interactions. The SMSS Maestro program allows for identification of these interactions based on geometrical conditions. The identified π-π interactions between CT and EH are illustrated in Figure 3, in which the mentioned interactions are visualized as blue dashed lines.

The results presented in Figure 3 indicate that the highest number of π-π interactions formed in the

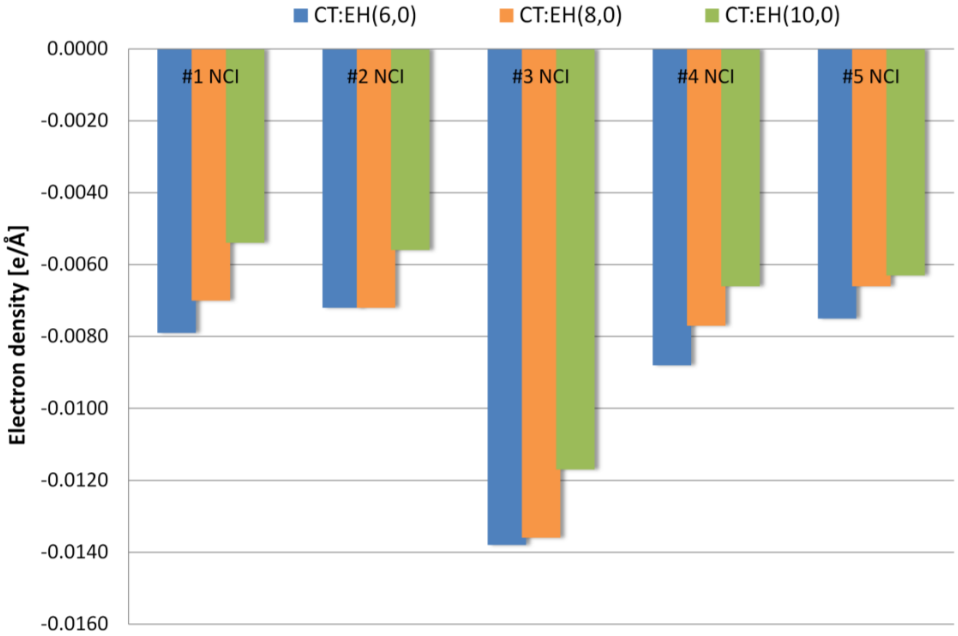

Figure 2. *The strength of NCIs expressed in terms of electron density.*

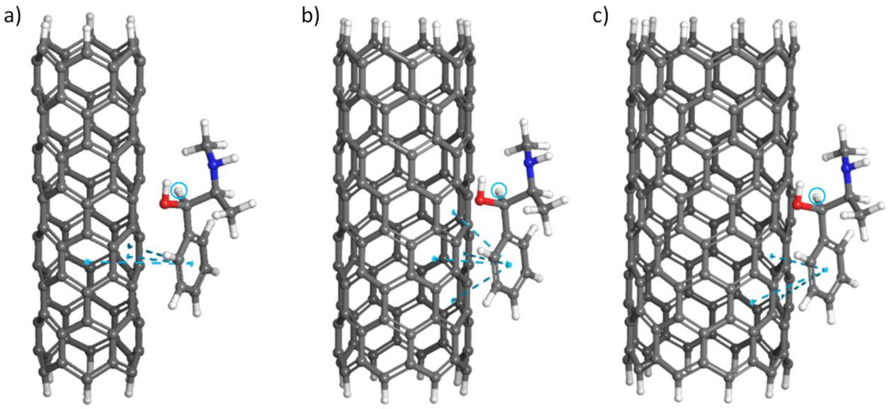

Figure 3. *Identified π-π interactions between CTs and EH a) CT:EH(6,0), b) CT:EH(8,0), c) CT:EH(10,0) systems.*

case of the CT:EH(8,0) system, the same one characterized by the highest binding energy. In this particular case, four π-π interactions formed, while in the remaining two cases, three π-π interactions formed. It is reasonable to guess that a higher number of π-π interactions contributes to the higher binding energies between CT and EH.

3.4. Molecular electrostatic potential surfaces

The reactivity of the system, which consists of CT and EH, can be analyzed through the analysis of the charge distribution, which provides valuable information on how molecular structures might interact with other structures. The charge distribution was analyzed through the molecular electrostatic potential (MEP).

To understand how charge distribution changes after the adsorption of EH by CT, we have calculated the MEP of individual structures and compared them with the MEP of CT:EH systems. The lowest and highest MEP values of individual structures are presented in Table 1, while MEP values of CT:EH systems were mapped to the electron density surface, which is how the MEP surfaces are obtained (Figure 4).

Table 1. *The lowest and highest MEP values of individual structures.*

MEP [kcal/mol]/ System	EH	CT(6,0)	CT(8,0)	CT(10,0)
Lowest value	–35.93	–16.73	–12.45	–12.28
Highest value	–32.39	41.41	33.77	29.44

The lowest and highest MEP values of individual structures presented in Table 1 indicate that in terms of the negative values, EH is much more reactive than the considered CT adsorbers. Namely, EH is characterized by the lowest MEP value of –35.93 kcal/mol. Of all CTs considered in this work, the lowest MEP value has been calculated for the lowest-diameter one - CT(6,0). This CT is characterized by the lowest MEP value equal to –16.73 kcal/mol. Larger considered CTs, CT(8,0) and CT(10,0), have a significantly lower magnitude of the negative MEP, equal to –12.45 kcal/mol and –12.28 kcal/mol, respectively. The highest positive values of the MEP in the case of CTs will not be considered, as they belong to hydrogen atoms that have been used only for the termination of CTs.

Results presented in Figure 4 show that the significant charge transfer occurred due to the EH adsorption by CT and that the highest amount of charge transfer happened in the case of the adsorption of EH by CT(6,0). In all cases, the values represented by the MEP colors indicate charge transfer. Namely, in CT:EH systems, the red color of MEP denotes the lowest values. In the case of the CT:EH(6,0) system, the red color denotes the values of –43.88 kcal/mol, while for the EH alone, the lowest MEP value was –35.93 kcal/mol. This difference indicates that upon the adsorption of EH by CT(6,0), the vicinity of the oxygen atom of EH gained in electron density. The same occurred in the cases of CT:EH(8,0) and CT:EH(10,0), however, to a lower extent, since in these cases, the red color of MEP denotes the values of –37.46 kcal/mol and –38.76 kcal/mol, respectively. Therefore, the lower amount of charge transfer occurred in the case of the larger diameter CTs.

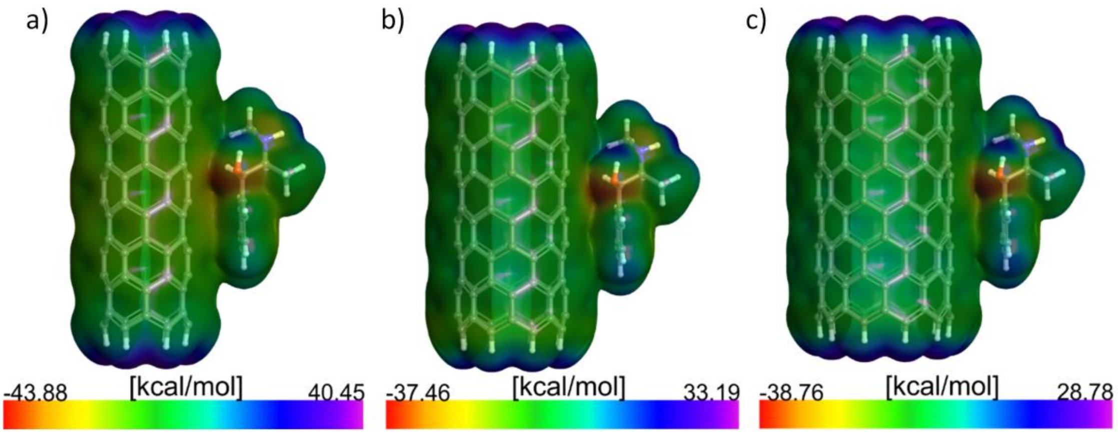

Figure 4. *MEP surfaces of CT:EH complexes a) CT:EH (6,0), b) CT:EH (8,0), and c) CT:EH (10,0).*

CONCLUSION

In this work, DFTB and DFT calculations were used to investigate the adsorption of EH using three representative CT models. Due to the size of the considered systems, DFTB calculations have been used to optimize all structures. DFT calculations on optimized structures were used to calculate binding energies. To identify NCI formed between the EH and CTs, periodic structures were transferred to molecular configuration, after which the electron density between atoms was analyzed. In all cases, the strongest NCI involved the EH's hydrogen atom in the vicinity of the oxygen atom. In this particular case, the strength of NCI is almost two times higher than any other NCI formed between EH and CT with the values ranging from –0.017 to –0.0138. The highest number of π-π interactions occurred in the CT:EH(8,0) system, the same system characterized by the strongest binding energy of –0.53 eV, confirm significant non-covalent interactions between CTs and EH. Finally, the analysis of MEP surfaces indicated that the highest amount of charge transfer occurred in the case of the EH adsorption by CT(6,0) wherein the MEP value was –43.88 kcal/mol. The results highlight CTs' strong potential to adsorb EH molecules with significant binding energies, balancing adhesion and desorption under realistic conditions. These findings provide valuable insights into CT-EH interactions and support the use of CTs in environmental remediation of pharmaceutical pollutants.

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ISTRAŽIVANJE ADSORPCIJSKOG POTENCIJALA UGLJENOVIH NANOCEVI KAO EFIKASNIH ADSORBORA ZA MOLEKULE LEKOVA

Sažetak: Ovaj rad se bavi istraživanjem interakcije između ugljeničnih nanocevi (CT) i molekula efedrina (EH) kroz sveobuhvatno korišćenje teorije funkcionalne gustine (DFT) i proračuna funkcionalne gustine vezivanja (DFTB) primenjenih i na periodične i na izolovane strukture. EH, kao široko rasprostranjena farmaceutska zagađujuća supstanca, stupa u interakciju sa CT i istaknutim organskim nanostrukturama, što podstiče pažljivo ispitivanje CT potencijala kao EH adsorbenata. Višestruki CT modeli su sistematski ispitani da bi se detaljno razjasnila njihova interakcija sa EH. S obzirom na značajnu složenost sistema koji uključuju 122–187 atoma, DFTB metodologija je korišćena za geometrijske optimizacije. DFT proračuni su naknadno korišćeni za dobijanje tačnih ukupnih energija, omogućavajući preciznu procenu energija vezivanja između EH i nanocevi. Energije vezivanja, u rasponu od -0,46 eV do -0,53 eV, potvrđuju značajne nekovalentne interakcije između CT i EH. Najkraća udaljenost između EH i CT u svim posmatranim sistemima uključuje atom vodonika u blizini atoma kiseonika što je takođe ključno za nekovalentne interakcije. Rezultati naglašavaju sklonost CT nanocevi da adsorbuju EH molekule sa značajnim energijama vezivanja, stvarajući ravnotežu između robusne adhezije i olakšavanja desorpcije pod verovatnim eksperimentalnim uslovima. Ovi rezultati ne samo da bacaju svetlo na osnovne mehanizme koji upravljaju interakcijom CT-EH, već nude i obećavajući uvid za praktičnu primenu CT nanocevi u strategijama obnove životne sredine koje ciljaju na farmaceutske zagađujuće supstance.

Ključne reči: Farmaceutik, DFT, energije vezivanja, remedijacija životne sredine.

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