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Research Article

# Theoretical study of drug delivery through drug adsorption on nanocarriers using density functional theory (DFT) method

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## ABSTRACT

This study investigates the adsorption of the drug hydralazine onto a zigzag single-walled carbon nanotube, CNT (9,0), using density functional theory (DFT) calculations at the B3LYP/6-31+G* level. Optimized structures, adsorption energies, frontier molecular orbital (HOMO–LUMO) characteristics, electronic density of states (DOS), and thermodynamic parameters were evaluated. The results indicate that hydralazine binds to the nanotube through nitrogen atoms with $sp^3$ hybridization, producing relatively high adsorption energy (−26.3 kcal/mol) and a reduced energy gap, both of which suggest enhanced stability. Analysis of bonding interactions, adsorption energetics, and electronic properties supports the conclusion that hydralazine adsorption on CNT (9,0) could enhance drug efficiency and enable selective cellular targeting. Therefore, CNT (9,0) shows strong potential as a nanocarrier for hydralazine in targeted drug delivery systems.

***Keywords*:** Single-wall carbon nanotubes (SWCNTs), Hydralazine, HOMO-LUMO, density functional theory (DFT), adsorption energy

## 1. Introduction

With the advancement of nanotechnology, the application of nanostructures in medicine, particularly in targeted drug delivery, has attracted significant attention. Carbon nanotubes (CNTs), owing to their unique properties such as high surface area, chemical stability, excellent conductivity, and the ability to be surface-functionalized, are considered among the most promising nanocarriers for drug delivery[1].

Hydralazine, a vasodilator widely prescribed for the treatment of hypertension, heart failure, and pregnancy-induced hypertension, is limited by low bioavailability, a short half-life, and adverse effects including tachycardia, headache, and nausea. These shortcomings underscore the need for advanced formulations to achieve targeted delivery [2-4]. In this context, the use of carbon nanotubes can serve as an effective platform to enhance solubility, reduce the required dosage, and improve the therapeutic efficacy of the drug [5].

The main objective of the present study is to theoretically investigate the adsorption of hydralazine molecules on CNT (9,0) and to evaluate the stability, reactivity, and electronic properties of the complex using density functional theory (DFT) calculations. In recent years, the preparation of nanoparticles as carriers for drug delivery has attracted considerable attention [6].

These nanoparticles can encapsulate and protect drugs while ensuring their delivery to the desired site [7-9]. Nanotechnology can enable drugs to reach target cells more specifically, thereby preventing the occurrence of side effects [9, 10]

In smart drug delivery systems, drugs are selectively loaded onto nanocarriers. These nanoparticles exhibit unique characteristics such as small size, large surface area, and tunable physicochemical properties that enable the targeted delivery of therapeutics to specific sites in the body [11, 12].

Pristine carbon nanotubes have highly hydrophobic surfaces, which can promote aggregation and unwanted interactions with other molecules. Functionalization makes them more hydrophilic, thereby improving water solubility, enhancing biocompatibility, and potentially reducing toxicity [13-15]. Carbon nanotubes can penetrate cell membranes and be internalized, enabling them to traverse various cellular compartments, including the nucleus [16].

Over the past two decades, carbon nanotubes (CNTs) have attracted significant attention as emerging carriers in drug delivery systems. In particular, single-walled carbon nanotubes (SWCNTs), with their hollow structures and nanometer-scale diameters, can effectively transport drugs, biomolecules, and even genes. Their high surface area, ability to penetrate tissues, electrical conductivity, and chemical stability make SWCNTs highly promising candidates for targeted drug delivery [1, 17].

A study by Xu and colleagues demonstrated that carbon nanotubes can achieve effective adsorption of cyclic drugs through π–π interactions. This type of noncovalent interaction allows for controlled drug release under biological conditions without chemically altering the drug[13].

In this context, Hashemzadeh et al. showed that PEG-functionalized carbon nanotubes exhibit improved aqueous dispersibility and reduced cytotoxicity [17].

Furthermore, Moradi's study on the adsorption of anticancer drugs such as chlorambucil, cyclophosphamide, and melphalan on CNT(9,9) demonstrated that the adsorption energy of these drugs is directly related to the nanotube structure, and that encapsulated systems exhibit greater stability under biological conditions [18].

Theoretical approaches, particularly density functional theory (DFT), enable the simulation of drug–nanocarrier interactions and prediction of molecular behavior. Taherpour et al. demonstrated that the adsorption site and orientation of a drug on SWCNTs critically affect complex stability, highlighting DFT's value for screening nanocarriers when experiments are time-consuming or costly [19].

DFT calculations have also been used to study metformin adsorption on graphene, revealing that a decreased HOMO–LUMO gap upon adsorption enhances the complex's electronic reactivity, serving as a key predictor of nanocarrier effectiveness [20]. Hydralazine, with its aromatic structure, can engage in π–π interactions with nanostructures, but its low bioavailability, metabolic instability, and short half-life necessitate formulation modifications [2, 3].

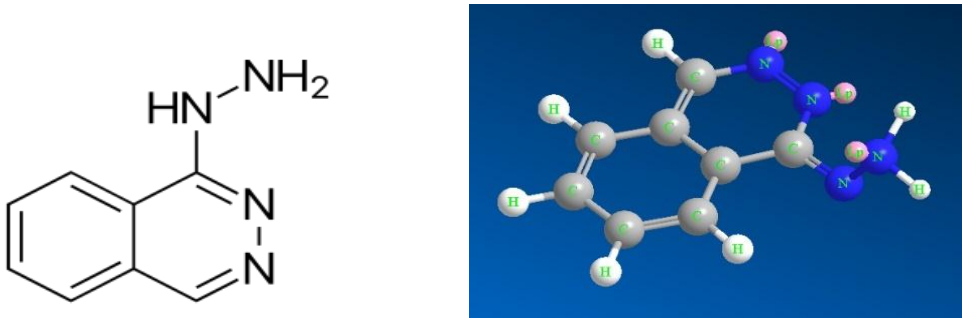



**Figure 1.** Chemical structures of hydralazine

The few studies conducted on controlled-release systems for hydralazine (Fig. 1) have mostly focused on biodegradable polymers or liposomes, while the role of carbon nanotubes has largely been overlooked. This scientific gap provides the primary motivation for the present study, which aims to theoretically investigate the adsorption of hydralazine on CNT (9,0) and to provide valuable insights into the stability, electronic structure, and thermodynamic properties of the resulting complex.

Although various studies have been conducted on the adsorption of common drugs on nanostructures such as graphene, fullerene, and carbon nanotubes [21-24], However, prior to this study, no theoretical investigation had been conducted on the interaction of hydralazine with CNT (9,0) carbon nanotubes. Another advantage of the present research is the use of precise DFT data to extract thermodynamic parameters such as adsorption energy, dipole moment, chemical hardness, and density of states, enabling scientific comparison with similar systems. These studies have demonstrated the significance of carbon nanotubes in drug delivery, yet a detailed examination of hydralazine adsorption on CNT (9,0) has not been performed, which this research aims to address.

## 2. Materials and Methods

The Gaussian 09W computational framework was employed for conducting quantum chemical computations in this investigation [25, 26]. In this study, the molecular structure of hydralazine (Figure 3-1) and the CNT(9,0) carbon nanotube were constructed using GaussView and Nanotube Modeler software, and subsequently optimized at the B3LYP/6-31+G* level using Gaussian 09 [27].

(a) (b)

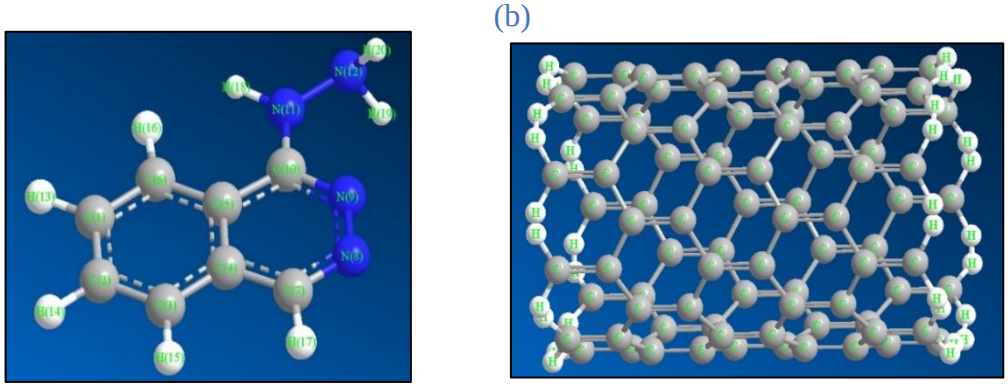


**Figure 2 .** Structure of Hydralazine (a) and CNT (9,0) (b)

As shown in Figure 3, two different structures of the drug–nanotube complexes were designed and analyzed.

(c) (d)

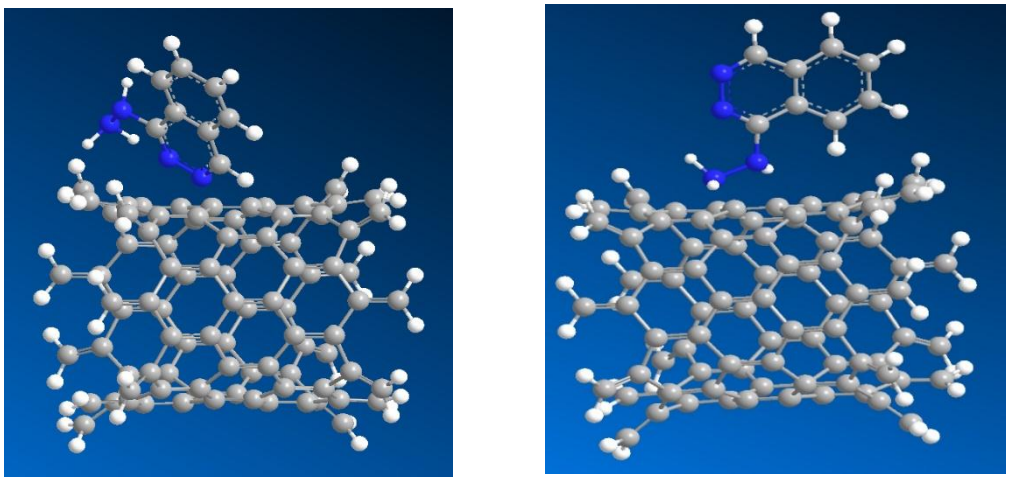


**Figure 3.** Optimized structure of the hydralazine–carbon nanotube complex (c-d)

The following parameters were investigated to compare the structures:Adsorption energy ($E_{ad}$)

- Dipole moment
- HOMO–LUMO energy gap
- Electronic density of states (DOS)
- Fundamental properties (chemical potential, electronegativity, hardness, and softness)

All calculations were performed without imposing any constraints on the geometric structures.

### *2.1. Modeling of the initial structures*

In the first step, the molecular structure of hydralazine (molecular formula $C_8H_8N_4$) and the zigzag carbon nanotube (CNT (9,0)) were modeled. The primary structure of the drug was drawn and optimized using GaussView software. The nanotube structure was generated using Nanotube Modeler. The modeled nanotube consists of 9 ring rows (chiral vector 9,0) with an approximate length of 10.6 Å and a radius of 3.6 Å, comprising 90 carbon atoms. Hydrogen atoms were added at both ends to saturate the edges and prevent edge effects.

Quantum chemical calculations were performed using the Gaussian 09 software package. The geometries of the drug, the nanotube, and the two drug–nanotube complexes were optimized separately. The B3LYP hybrid functional (Becke, 3-parameter, Lee–Yang–Parr) in combination with the 6-31+G* basis set was employed to describe the electron density, providing a suitable balance between accuracy and computational cost. All calculations were carried out in the gas phase with a closed-shell spin configuration. No constraints were applied to the geometric parameters, and the structures were fully optimized without restrictions.

### *2.2. Optimization of the complex structures*

Two different configurations of hydralazine adsorption on the nanotube were considered:

- Complex 1: The drug is positioned flat and parallel to the nanotube surface, allowing for strong π–π interactions.
- Complex 2: The drug is oriented at an angle relative to the nanotube axis, located at a different position with respect to the center of the nanocarrier.

The geometries of both complexes were optimized separately to obtain their stable structures. The distance between the drug's center of mass and the nanotube surface was set in the range of 3.2–3.6 Å, consistent with typical noncovalent van der Waals and π–π interaction distances.

### *2.3. Calculation of adsorption energy*

To evaluate the stability of the complexes, the adsorption energy was calculated using the following equation:

$$E_{ads} = E_{product} - [E_{drug} + E_{CNT}] \qquad \text{(Eq.1)}$$

where:

- $E_{product}$: total energy of the drug–nanotube system
- $E_{CNT}$: optimized energy of the nanotube
- $E_{drug}$: optimized energy of the hydralazine molecule

A negative adsorption energy indicates stable and spontaneous binding of the drug to the nanocarrier. The adsorption energies were calculated and compared for both complex structures.

**Table 1.** Absorption energy ($E_{ads}$), HOMO and LUMO energies, and energy gap ($E_g$) before and after the placement of hydralazine on the nanotube.

| Structures | $E_{ads}$ (kcal/mol) | HOMO (eV) | LUMO (eV) | Eg (eV) |
|---|---|---|---|---|
| Hyd (a) | - | −5.61 | −1.38 | 4.23 |
| CNT (9,0) (b) | - | −6.56 | −0.95 | 5.61 |
| CNT (9,0) and Hydr (c) | −18.7 | −5.82 | −2.20 | 3.62 |
| CNT (9,0) and Hydr (d) | −26.3 | −5.72 | −2.27 | 3.45 |

Numerically, Complex d, with an adsorption energy of −26.3 kcal/mol, exhibited greater stability compared to Complex c, which had an adsorption energy of −18.7 kcal/mol. These values indicate that Complex d possesses higher thermodynamic stability, and drug adsorption in this configuration is not only energetically favorable but also spontaneous and stable. The large negative adsorption energy suggests that the drug binding is thermodynamically spontaneous and stable, and it may effectively compete with other proposed carriers.

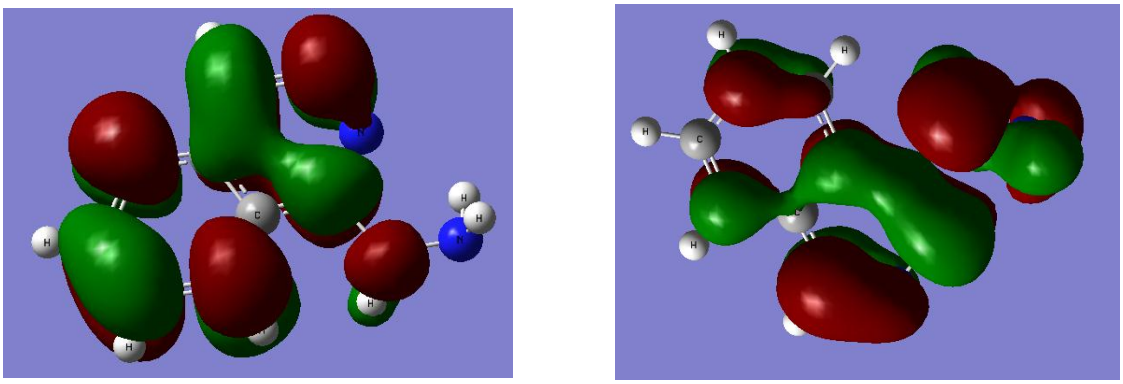
Analysis of the optimized structures of the drug–nanotube complexes revealed that in both modeled configurations, drug adsorption occurs via physical, noncovalent interactions, particularly π–π stacking. Unlike chemisorption, this type of adsorption does not disrupt the structure of either the drug or the carrier, thereby enabling reversible and controlled drug release.

### *2.4. HOMO–LUMO orbital calculations*

To analyze the chemical reactivity and electronic stability of the system, the energy levels of the frontier molecular orbitals HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) were examined [28] (Fig 4-5).The energy gap between these two orbitals ($E_{gap}$) was calculated using the following equation:

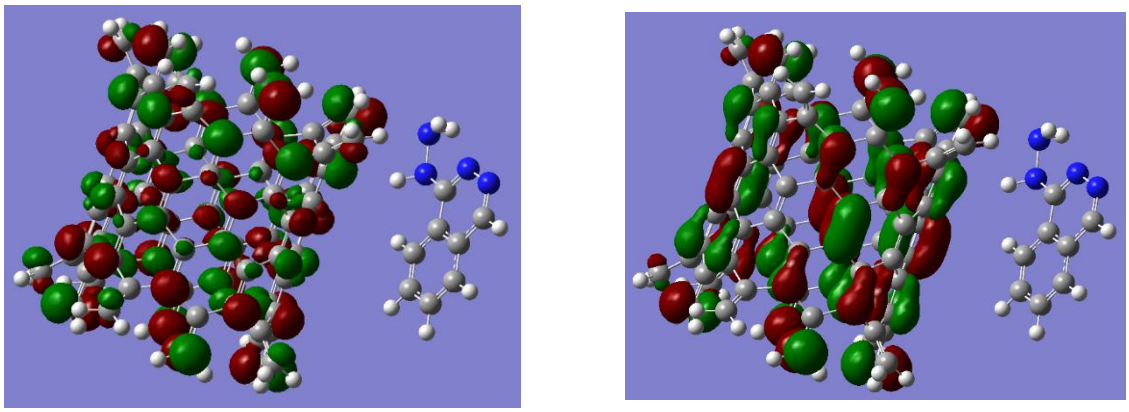
$$E_{gap}=E_{LUMO}-E_{HOMO} \qquad \text{(Eq.2)}$$

A decrease in the HOMO–LUMO energy gap is generally associated with increased electronic reactivity and conductivity. Orbital density analysis was performed using GaussView outputs. The HOMO–LUMO energy gap is a key parameter for evaluating the reactivity of molecular systems. Comparison of the gaps for the pristine nanotube, the drug, and the resulting complexes revealed that drug adsorption reduces the system's energy gap. This effect is particularly pronounced in Complex d (3.45 eV), indicating enhanced electronic conductivity and chemical reactivity following adsorption. Such characteristics may play a significant role in targeted drug activation or responsiveness under specific biological conditions.



LUMO HOMO

**Figure 4.** HOMO and LUMO orbitals of the hydralazine molecule



LUMO HOMO

**Figure 5.** HOMO-LUMO orbitals of the CNT (9,0) nanotube + Hydralazine complex, Structure (d)

### *2.5. Density of states (DOS) analysis*

To better understand the electronic structure and electron density redistribution in the complexes, the density of states (DOS) spectra was generated using GaussSum 3.0 [29] (Fig 6-7). These spectra allow visualization of the proximity of energy states to the Fermi level and their distribution within the system. Changes in the density of states around the Fermi energy (E-F) can indicate strong electronic interactions between the drug and the nanocarrier. The DOS spectra were plotted to examine the electronic behavior of the systems. In the pristine CNT, the density of states is symmetrically distributed around the Fermi level (E-F). However, after drug adsorption:

- In Complex d, new states appeared near the Fermi level.
- These changes indicate strong orbital interactions and an increased likelihood of electron transfer between the drug and the nanocarrier.

From an application perspective, this feature may facilitate controlled electronic release of the drug under biological conditions.

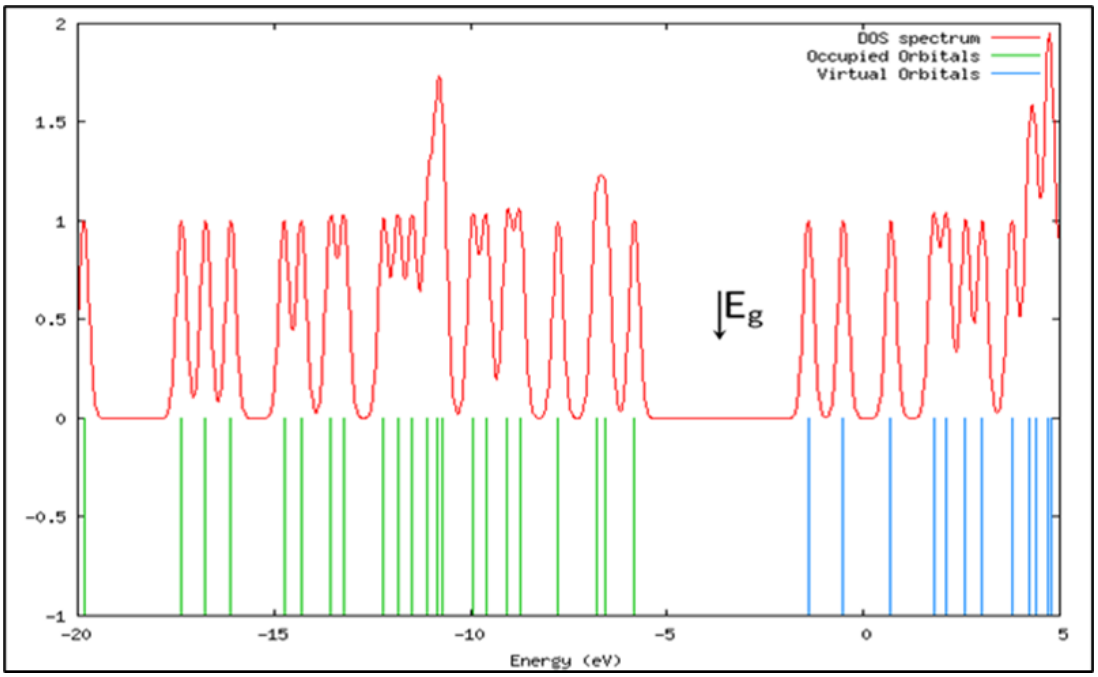
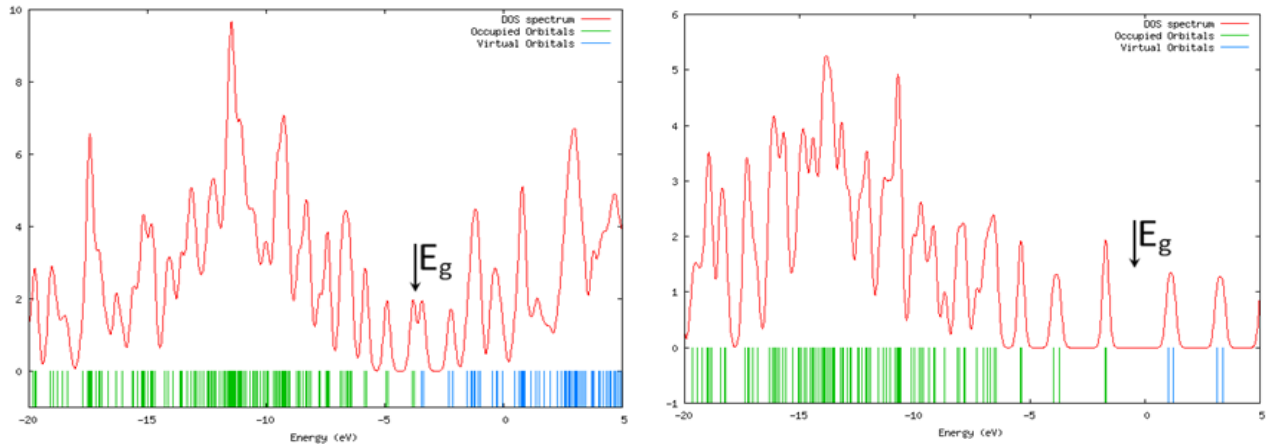



**Figure 6.** DOS spectrum of the hydralazine molecule




CNT (9,0) and Hydrazine (d) CNT (9,0)

**Figure 7.** DOS spectrum of the CNT (9,0) nanotube and CNT (9,0) nanotube + Hydralazine complex, Structure (d)

### *2.6. Dipole moment and system polarity*

The dipole moment values of the systems were also examined as indicators of polarity and solubility potential (Table 2). The dipole moments were analyzed to assess how the molecular polarity changes as a result of drug adsorption.

**Table 2.** Dipole moment of the structure before and after adsorption of Hydralazine onto the nanotube calculated using B3LYP/6-31+G*

| | X | Y | Z | total |
|---|---|---|---|---|
| Hyd (a) | -0.7493 | 2.3666 | 0.7681 | 2.5985 |
| CNT (9,0) (b) | 0.7477 | -1.0770 | -1.2110 | 1.7848 |
| CNT (9,0) +Hydr (c) | 4.7533 | -2.1900 | -0.4339 | 5.2515 |
| CNT (9,0) + Hyd (d) | -5.6175 | -2.0094 | 0.9741 | 6.0451 |

The significant increase in dipole moment observed in both complexes indicates an enhancement of the system's polarity after drug adsorption. This increase can improve the complex's solubility in aqueous environments and enhance the bioavailability of the drug under physiological conditions.

### *2.7. Fundamental properties*

The ionization potential (I), electron affinity (A), chemical potential (μ), hardness (η), and softness (σ) of Complexes 1 and 2, as well as of the hydralazine molecule and CNT (9,0)

nanotube before and after binding, were calculated using the following equations and are presented in Table 3.

$$I = -E_{HOMO} \quad \text{(Eq.3)}$$

$$A = -E_{LUMO} \quad \text{(Eq.4)}$$

$$\mu = -\frac{1}{2}(I + A) \quad \text{(Eq.5)}$$

$$\eta = \frac{1}{2}(I - A) \quad \text{(Eq.6)}$$

$$\sigma = \frac{1}{\eta} \quad \text{(Eq.7)}$$

These parameters were calculated based on equations derived from conceptual DFT using the HOMO and LUMO energies. These properties play a crucial role in predicting drug release behavior and chemical interactions with the biological environment.

**Table 3.** Fundamental properties of the structure before and after adsorption of Hydralazine onto the nanotube calculated

| structure | I (ev) | A (ev) | μ (ev) | η (ev) | σ(ev) |
|---|---|---|---|---|---|
| Hyd | 5.83 | 1.4 | −3.495 | 2.22 | 0.45 |
| CNT (9,0) | 1.67 | -1.02 | -0.33 | 1.35 | 0.74 |
| CNT (9,0) and Hyd (c) | 3.78 | 4.44 | −4.01 | 1.81 | 0.552 |
| CNT (9,0) and Hyd (d) | 3.72 | 4.64 | −4.00 | 1.725 | 0.579 |

Compared to the pristine CNT, both complexes exhibit lower hardness (indicating higher reactivity), greater softness (increased tendency for interaction), and higher electronegativity. These changes indicate enhanced electronic stability, reduced resistance to structural deformation, a greater propensity for electron uptake, and increased reactivity of the complexes relative to the pristine nanotube.

## 3. Conclusion

Nowadays, carbon nanostructures have attracted considerable attention as nanocarriers due to their small size, high surface-to-volume ratio, biocompatibility with living cells, presence of active functional groups, and favorable interactions with drug molecules, making them promising candidates for advanced drug delivery systems.

In this study, the interaction of the antihypertensive drug hydralazine with a zigzag single-walled carbon nanotube (CNT (9,0)) was investigated using a theoretical approach based on density functional theory (DFT). The aim of this research was to evaluate the thermodynamic stability, electronic properties, and theoretical potential of CNTs as nanocarriers for targeted delivery of hydralazine. Based on the structural, electronic, and thermodynamic results obtained in this study, the following conclusions can be drawn:

- The CNT (9,0) carbon nanotube exhibits a high structural and electronic capacity for adsorbing hydralazine.
- Drug adsorption occurs via noncovalent and stable interactions, leading to enhanced conductivity and reactivity of the complex.
- The properties observed in Complex d (smaller energy gap, higher adsorption energy, better charge transfer) make it the optimal candidate for hydralazine delivery.
- Structural optimization of hydralazine, the CNT (9,0) nanotube, and the resulting complexes revealed two possible adsorption configurations: in the first (Complex d), the drug lies horizontally and parallel to the nanotube surface, while in the second (Complex c), the drug is adsorbed at an angle and further from the surface. Geometric analysis indicated that in Complex d, the distance between the aromatic ring of the drug and the nanotube surface is approximately 3.4 Å, reflecting a stable π–π interaction between the two structures.
- In this configuration, the drug has maximum contact with the nanotube, enhancing the stability of the complex. In contrast, in Complex c, the drug occupies a less stable position at an angle to the nanotube axis, resulting in reduced contact area between the two structures.

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