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The sensing behavior of MgO nanotube to thiopropamine drug via DFT investigation

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ABSTRACT

This work mainly aimed to develop a sensor based on MgO nanotubes (MgONTs) to detect thiopropamine (TP) using density functional theory (DFT). The abuse of drugs has major negative effects, and measures are to be implemented throughout the world to detect and control illegal drugs, e.g., TP. As a result, it is necessary to detect the TP drug in biological settings. The sensing characteristics of MgONTs for TP detection purposes were evaluated using DFT. MgONTs were found to have remarkable reactivity toward TP molecules and had a sensing response of 298.11. In addition, the HOMO and LUMO energy levels and therefore, the energy gap were significantly shifted by TP adsorption. The reduced energy gap was observed to raise electrical conductivity. The recovery time was short for TP desorption from the MgONT surface (nearly 18.67 ms). It can be said that MgONTs can be both efficient and effective electronic sensors of TP and a promising drug delivery system (DDS) for the TP drug in biological applications.

1. Introduction

It is crucial to detect and control illegal drugs since their abuse has major consequences [1-7]. The abuse of thiopropamine (TP) imposes dramatic negative effects. Hence, TP must be detected in biological settings [8-10]. Drug abuse can also lead to mental conditions [7, 11-15]. Hence, it is necessary to develop simple, affordable, and responsive sensors of significant sensitivity and accuracy to detect TP. Nanomaterials have been comprehensively used in various biological fields, such as biosensing, cell targeting, drug delivery, and bioimaging. [16-28].The use of nanomaterials to deliver anticancer drug molecules to tumorous tissues remains a major challenge [29-33]. Nanostructured drug delivery systems (DDSs) have resulted in an intracellular treatment [34-39]. Extensive research has been reported on the analysis of nanosheets, nanotubes, and nanoclusters in chemical sensor development in light of their major advantages over conventional sensors, including large surface-volume ratios [40-49]. Numerous studies investigated the applications of nanostructured systems consisting of elements in groups II to V. There are substantial concentrations of MgO in salt rocks. MgO possesses high chemical and thermal stability and can be employed for a wide variety of purposes, including refractory materials and catalytic agents [52,53]. MgO particles have been of significant interest to researchers. They have a large unique surface area up to 500 m^2/g and the average size of their crystals is 4 nm [54]. MgO particles could be efficient adsorbents in light of their large specific surface area and great surface reactivity [55]. Researchers have experimentally [56,57] and theoretically [58-60] studied

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MgO nanoclusters. Ziemann and Castleman [58] introduced the stable cubic MgO structure. Furthermore, MgO nanobelts, metal oxide nanowires, nanofilms, and nanorods have been reported [61-63]. The more recent forms of MgO include single-walled carbon nanotube (CNT)-improved MgO layers, Ga-filled MgONTs, and MgO nanotube bundles [64-66] with several potential applications. Several studies recently analyzed the constructional, electronic and adsorption properties of MgO and the interaction between MgO and single molecules [67,68]. Earlier works reported that MgONTs have a state energy of 0.12-0.66 eV (more than that of cage and cubic isomers) [69]. Valero and Yang [70] studied CO adsorption onto MgONTs. Beheshtian [71] analyzed the interaction of NO and CO molecules with the MgONT surface using DFT. They reported the strong adsorption of NO and CO gases onto MgONTs with a remarkable adsorption energy value. Peyghan et al. [72] studied N_2O adsorption into MgONTs and showed that the pristine MgONT surface could not be a strong adsorbent of N_2O. Ammar [73] reported the NO strong adsorption onto the MgONT surface, with an oxygen vacancy. Following the works proposing MgONT as a superb sensor for the detection of pollutants such as CO, NO, CO_2, SO_2, NH_3 and NO_2, it remains yet to realize whether MgONT can be used for TP drug detection. To the best of the authors, the detection of TP molecules using MgONT adsorption systems has not been numerically studied. Therefore, the present work seeks to analyze the interaction of TP molecules with the MgONT surface to measure the potential use of MgONTs for the adsorptive sensing of TP. The sensing properties and the adsorption energy were analyzed using DFT.

2. Computational details

The current study executed the calculations in GAMESS [74] and carried out a density of state (DOS) analysis using GaussSum [75]. The TPSS functional is efficient for accurate electronic and structural evaluations of metal complexes [76,77]. It was employed with the 6-311G (d) basis set for the electronic, charge transfer, energetic, and structural analyses. Grimme's "D" term was also adopted for dispersion correction in the TPSS functional [76]. The counterpoise procedure has been used to obtain the basis set superposition error (E_{BSSE}) error [78]. The adsorption energy (E_{ad}) is written as:

$$E_{ad} = E_{(drug/MgONT)} - E_{(drug)} - E_{(MgONT)} + E_{BSSE} \quad (1)$$

where $E_{(drug/MgONT)}$ is the TP/nanotube complex energy, while $E(drug)$ denotes the isolated drug molecule energy.

3. Results and discussion

A MgONT structure with a total length of 14.79 Å, five polygons, and seventy-two atoms was employed. The initial polygons showed a small planarity difference. Wilson [79] used an empirical compressible ion potential model and introduced identical and slightly distorted MgONT structures. Figure 1 shows the optimized structures and DOS plot. Two Mg–O bonds were identified, one with a length of 1.90 Å and the other one with a length of nearly 1.95 Å. The latter bond was parallel with the axis of the MgONT. However, the length of the diagonal bonds was equal to 2.03 Å by the PBE function and 2.01 Å by the TPPS function [80]. Kakkar et al. [80] reported an average Mg–O bond length of approximately 1.975 Å in the internal zone and 1.994 Å in the external zone (0.02 Å longer external bong length). It is worth mentioning that the dipole moment of the bare MgONT is 0.15 Debye. 1.23|e| charge transfer from Mg to O has been observed by the ESP charge analysis, suggesting an extremely ionic system [81].

3.1. Structural analysis of TP/MgONT

As be seen in Fig. 2, a TP molecule consists of 2 nucleophilic groups, i.e., S and NH_2. These groups are assumed to be candidates for attacking MgONTs. The TP molecule was attached from the nucleophilic terminals to Mg atoms on the adsorbent surface. Figure 3 depicts the partial structures. This study estimated two relative minima to avoid process complication. In the most stable complex, TP molecules reacted through their N heads with an Mg atom on the adsorbent surface, with $E_{ad} = -16.43$kcal/mol. The N-Mg bond length was estimated to be 2.171 Å. Furthermore, there was a natural bond orbital (NBO) charge transfer as large as 0.25 |e| from the adsorbate to the adsorbent. In complex B, however, TP adsorption onto the adsorbent surface occurred through the sulfur atom, with $E_{ad} = -5.11$ kcal/mol.

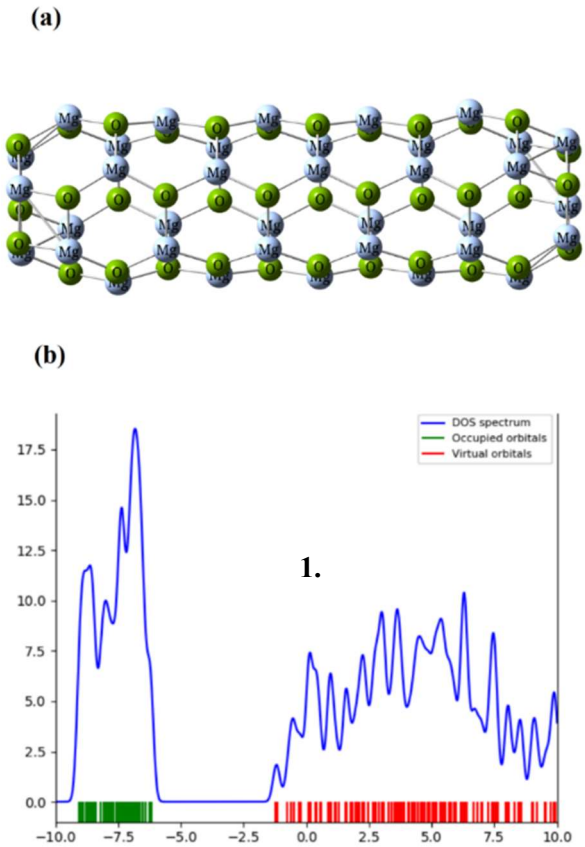

Fig. 1. *(*a) The optimized structure and (b) density of state (DOS) plot of MgONT.

Complex A had a stronger interaction than complex B. The repulsive forces between the partially positive Mg atoms of the adsorbent and the positively charged H head of the drug molecule could impose a remarkable challenge (i.e., steric hindrance) on TP adsorption. The adsorption of drug molecules onto the MgONT surface through its N atom leads to the minimization of this steric effect since N atoms carried a negative charge (pone pairs) toward Mg atoms. The single lone pair of the N atom is covered by a negative charge. When the N atom is attached to the adsorbent, the positive charge of the Mg atom is strongly attracted by the space charge of the N atom, and the steric effect is minimized. To electrically characterize the system, the net charge transfer from TP to MgONTs was analyzed in two complexes. The charge transfer to TP molecules was zero prior to the adsorption. A net charge transfer of 0.25 |e| in complex A and 0.062 |e| in complex B was measured. This implies that the direction of this charge transfer was from the adsorbate to the adsorbent. A number of DFT studies reported different behaviors in sensor systems toward various drugs in recent years [16, 82].

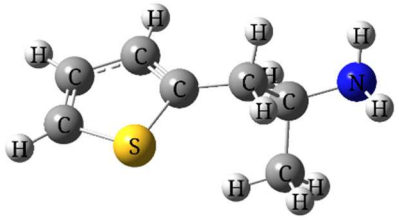

Fig. 2. Geometrical structure of the optimized TP drug.

3.2. Sensing mechanism

Resistivity variation following electron transfer between the adsorbate and adsorbent is a sensing mechanism determinant. The energy gap is related to the electronic change in MgONTs (and electrical resistance) as:

$$\sigma = AT^{3/2}\exp(-E_g / 2kT) \qquad (2)$$

where A is a constant ($e.m^{-3}k^{-3/2}$), whereas k denotes the Boltzmann constant. As can be seen, σ exponentially rises for the adsorbent as the energy gap reduces. This is explained by the existence of chemical factors. The sensor response (S) is experimentally calculated as:

$$S = |R_2 - R_1|/R_1 = |(R_2/R_1) - 1| \qquad (3)$$

where R_1 and R_2 denote the pre- and post-adsorption electrical resistance of MgONTs, respectively. There is a reverse correlation between electrical resistance and electrical conductivity. It can be inferred that a change in electrical resistance represents adsorption-induced energy gap variation MgONTs were reported to operate at ambient temperature [83].

$$S = |(\frac{\sigma_1}{\sigma_2}) - 1| = exp(|\Delta E_g|/kT) - 1 \qquad (4)$$

where ΔE_g represents the gap energy changes after the adsorption process. According to Table 1, TP in complex A dramatically changed the LUMO, HOMO, and Fermi levels and, therefore, the energy gap pristine MgONTs were estimated to have a sensing response of 298.11 toward TP at 298 K, representing substantial sensitivity.

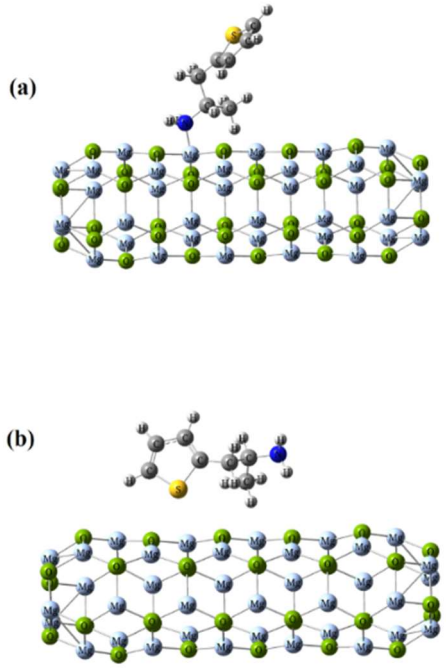

Fig. 3. Two various optimized structure of the MgONT/TP complexes.

3.3. Analysis of molecular orbitals

Figure 4 illustrates the HOMO and LUMO distributions of pristine MgONT structure and the most stable TP/MgONT structure. As can be seen, the HOMO and LUMO levels were frequently positioned near the electronegative (O and N) and electropositive (Mg) sites, respectively. The HOMO plots were mostly found on TP, whereas the LUMO levels were on MgONTs. This suggests that electrons had a higher density around O atoms. Hence, TP adsorption onto MgONTs changed the HOMO and LUMO levels (see Table 1). Furthermore, the tubular structure had the highest geometric stability obtained via 2p orbitals of O and 3s and 3p orbitals of Mg [84].

3.4. Recovery time

To experimentally evaluate the recovery time, the adsorbent is either heated or exposed to Ultra violet (UV) light [85]. The recovery time of TP/MgONT complexes was calculated as [86]:

$$\tau = \nu^{-1} exp^{(-\Delta G/kT)} \quad (5)$$

where υ signifies the attempt frequency whereas k and T indicate the Boltzmann constant and the temperature, respectively [85-88]. For an attempt frequency of 1018 s^{-1} under UV exposure, the recovery time was obtained to be 18.67 ms at 298 K. It was found that complex A had a rapid recovery. As a result, MgONTs could be a promising sensor of TP drug.

3.5. Solvent effect

The effect of water as a solvent on TP adsorption onto MgONTs was measured using the polarizable continuum model (PCM) [87]. The isolated TP, pristine MgONT, and complex A were re-optimized within the solvent. It was found that the solvent slightly weakened the TP-MgONT interaction, decreasing the adsorption energy to -14.23 kcal/mol.

Here, $\Delta E_{ad-sol-gas}$ denotes the difference between the gaseous and aqueous adsorption energy values.

$$\Delta E_{ad-sol-gas} = E_{ad-solution} - E_{ad-gas} = 2.20 kcal/mol \quad (6)$$

In particular, the solvation energy $\Delta E_{solvation}$ was estimated for the isolated TP, pristine MgONTs, and TP/MgONT system as:

$$\Delta E_{solvation} = E_{solution} - E_{gas} \quad (7)$$

where $E_{solution}$ shows the energy of the system in the aqueous medium, while E_{gas} indicates the energy of the system in the gaseous medium. The solvation energy was obtained to be -5.09 kcal.mol^{-1} for TP, -7.88 kcal.mol^{-1} for MgONTs, and -12.76 kcal.mol^{-1} for the TP/MgONT system. It can be said that TP and MgONTs are highly polar and water-soluble. As a result, H_2O molecules around the MgONTs and TP molecules weaken the TP-MgONT interaction.

Table 1. Estimated adsorption energy (E_{ad}) for TP drug adsorption on the MgO nanotube

Structure	E_{ad} (kcal/mol)	Q (e)	D (Å)	E_{HOMO} (eV)	E_{LUMO} (ev)	E_g (eV)	E_F (eV)	ΔE_g (%)
MgONT	–	–	–	− 6.43	− 2.84	3.59	− 4.63	–
Complex A	− 16.43	0.250	2.171	− 5.20	− 2.56	2.64	− 3.88	26.46
Complex B	− 5.11	0.062	2.453	− 6.11	− 2.63	3.48	− 4.37	3.06

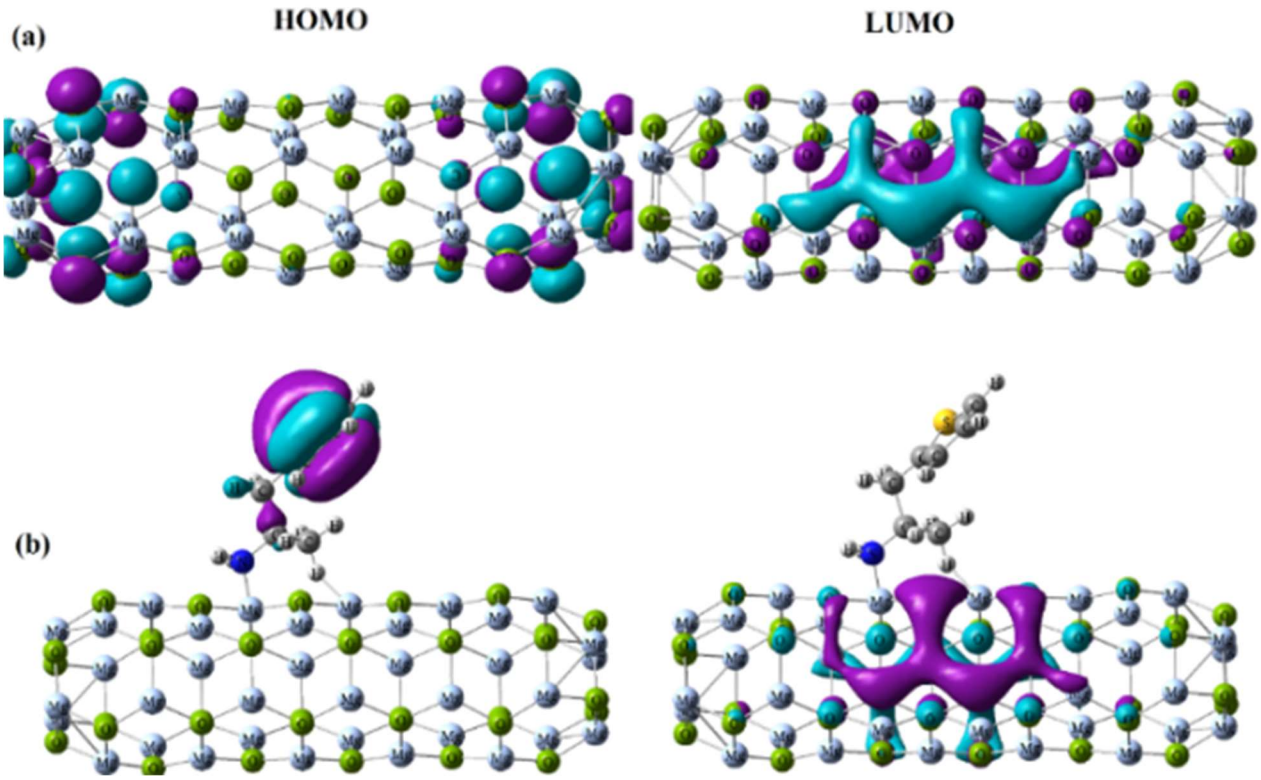

Fig. 4. The HOMO and LUMO figures of (a) MgONT and (b) most stable complex of MgONT/TP.

4. Conclusion

The 1D nanostructured systems possess remarkable electronic sensitivity toward a variety of chemical agents. This study implemented DFT to analyze the potential of MgONT for the sensing of TP drug. It was found that TP would chemisorbed onto the MgONT surface (E_{ad} = −16.43kcal/mol). The MgONT was estimated to have a sensing response of 298.11 toward TP molecules at 298 K. This is explained by the large charge transfer from TP molecules to MgONTs. In complex A, TP molecules reacted through their N heads with an Mg atom on the adsorbent surface, since Mg atoms have a small steric effect. Furthermore, MgONTs were estimated to have a rapid recovery for the desorption of TP molecules (18.67 ms). It was theoretically and numerically found that TP adsorption onto MgONTs would be modified by the electrical conductance of MgONTs. Therefore, MgONTs can be a promising biosensor of TP drug in medical settings.

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