CuO-decorated ZnO nanotube–based sensor for detecting CO gas: a first-principles study

Somayeh Tohidi1 · Tavakkol Tohidi2 · Parvin Hamdi Mohammadabad3

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Abstract
Understanding the effect of copper oxide (CuO)–decorated zinc oxide nanotube on carbon monoxide (CO) adsorption is crucial for designing a high-performance CO gas sensor. In this work, CO sensing properties of copper oxide–decorated zinc oxide (CuO-ZnO) nanotube are studied theoretically by employing first-principles density functional theory for the first time. The stability, adsorption mechanism, density of states, and change in electrical conductivity are studied. The results of calculating the adsorption energy show strong chemical adsorption of CO on CuO-ZnO nanotubes. The adsorption energy of CO on CuO-ZnO nanotube is calculated as 7.5 times higher than that on ZnO nanotube. The results of the Mulliken charge analysis reveal that electron transfer occurs from CO molecules to CuO-ZnO nanotubes. Additionally, the electrical conductivity of CuO-ZnO nanotubes significantly changes after adsorption of CO at room temperature. According to these studies, CuO-ZnO nanotube sensors can be used for the detection of CO gas. The results are in excellent agreement with the reported experimental results.

Keywords  Nano tube · Zinc oxide · DFT · Gas sensor · Electrical conductivity

Introduction
Carbon monoxide (CO) is a highly toxic, colorless, odorless, and tasteless gas. CO is a byproduct of the incomplete burning of fossil fuels with insufficient oxygen [1]. Exposure to a low concentration of CO (500 ppm) would lead to symptoms such as headache, dizziness, and nausea, whereas exposure to a higher concentration of more than 1500 ppm can result in death in most animate beings [2]. Therefore, CO gas detection is of great importance. Recently, various nanostructures have attracted extensive attention to develop sensing devices because of their high surface/volume ratio, good sensing performance, low-cost, and facility of miniaturization [3–14].

Zinc oxide (ZnO) is one of the most common nanostructures that has been extensively used in gas sensing devices due to its characteristics, such as superior electrical properties, chemical stability, and high electron mobility [15]. ZnO nanostructure has been reported to detect many hazardous gases, such as F2, NO2, NO, H2S, CO2, CO, triethylamine, ethanol, acetone, and chlorobenzene [16–22]. Nevertheless, pristine ZnO-based gas sensors had a weak interaction with different gas molecules. To solve this problem, some methods have been presented, including doping or decorating of impurity atoms, chemical functionalization, and introducing structural defects [23–25]. For example, Wei et al. [26] reported Pd-doped ZnO nanofibers with faster response and improved CO sensing. Lingmin et al. [27] showed that Al-doped ZnO nanovases exhibit four times better CO sensing response compared to the un-doped system.

However, it is a controversial issue to know how the doping or decorating of impurities changes the response of ZnO nanostructures in detecting CO. First-principles density functional theory (DFT) is a strong technique that can be utilized to explain the experimental results at the molecular level. For CO detection, a gas–solid interaction is needed to
change the electronic properties on the ZnO surface through charge transfer mechanism. Aslanzadeh [28] showed that V- and Cr-doped Zn$_{12}$O$_{12}$ nanoclusters have highly improved sensitivity to CO. Hadipour et al. [29] studied the adsorption of CO molecules on Al-doped ZnO nanoclusters. They found that C–Al bonds (1.95 Å and 2.07 Å) are formed with a remarkable decrease in the band gap energy. Here, for the first time, we perform a DFT study to investigate the adsorption of CO gas on CuO-decorated ZnO nanotubes. Moreover, different adsorption configurations of CO gas are considered. Charge transfer occurs between CO molecules and CuO-ZnO nanotube surface because of chemical adsorption.

**Methods**

These calculations were carried out based on the density functional theory by using a plane-wave base set and pseudopotential implemented in the Quantum Espresso package [30]. The generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) form was employed to compute the exchange–correlation energy–density functional. According to the Monkhorst–pack scheme, the Brillouin zone was sampled by $8 \times 1 \times 1$ k-point mesh for structural optimization. An energy cut-off of 80 Ry was utilized for the plane wave expansion to solve the Kohn–Sham equations. In all calculations, atomic positions were optimized until the convergence threshold on total energy (a.u) and forces (a.u) were $10^{-8}$ and $10^{-7}$, respectively. Moreover, the convergence threshold (conv-thr) for self-consistency (estimated energy error $< \text{conv-thr}$) was $10^{-10}$. An armchair single-walled nanotube structure was considered with 30 zinc atoms and 30 oxygen atoms.

CO and CuO get close to ZnO in three different orientations. Absorbance of each orientation is separately investigated in four positions. These four positions for absorbance of CO and CuO on ZnO nanotube include the following: top of zinc and oxygen atoms (Top or T$_1$-Type and T$_2$-Type), perpendicular to bond of the zinc-oxygen bond (Bridge or B-Type) and the center of the hexagonal structure of ZnO nanotube (Hollow or H-Type) as shown in Fig. 1A and B. Therefore, the 16 possible configurations with CO close to ZnO nanotube were as follows: a$_1$T$_1$, a$_2$T$_1$, a$_3$T$_1$, a$_4$T$_1$, a$_1$B, a$_2$B, a$_3$B, a$_4$B, a$_1$T$_2$, a$_2$T$_2$, a$_3$T$_2$, a$_4$T$_2$, a$_1$H, a$_2$H, a$_3$H, and a$_4$H. The 16 possible configurations with CuO close to ZnO nanotube were as follows: b$_1$T$_1$, b$_2$T$_1$, b$_3$T$_1$, b$_4$T$_1$, b$_1$B, b$_2$B, b$_3$B, b$_4$B, b$_1$T$_2$, b$_2$T$_2$, b$_3$T$_2$, b$_4$T$_2$, b$_1$H, b$_2$H, b$_3$H, and b$_4$H. Next, the most optimal configuration was chosen (the most stable configuration corresponds to a binding energy with the largest negative value).

CO gets close to CuO-ZnO nanotube in three configurations with the symmetry axis parallel and perpendicular to the plane in three configurations according to Fig. 1C. Three possible configurations in this case were as follows: C$_1$T, C$_2$T, and C$_3$T, so the most optimal configuration could be investigated (Fig. 1C).

The binding energy ($E_{\text{bind}}$) of all possible configurations of adsorption of CO and CuO molecules on ZnO nanotube was calculated by:

$$E_{\text{bind}} = E_{\text{total}} - (E_{\text{(ZnO nanotube)}} + E_{\text{molecule}})$$

where $E_{\text{total}}$ is the total energy of CuO adsorbed on ZnO nanotube, $E_{\text{(ZnO nanotube)}}$ is the total energy of the ZnO nanotube, and $E_{\text{molecule}}$ is the total energy of free CO or CuO molecules. Moreover, to find the binding energy, $E_{\text{bind}}$ between CO and CuO-ZnO nanotube structure (CO/CuO-ZnO nanotube), the following equation was used:

$$E_{\text{bind}} = E_{\text{total}} - (E_{\text{(CuO-ZnO nanotube)}} + E_{\text{CO}})$$

where $E_{\text{total}}$ is the total energy of the CuO-ZnO nanotube structure interacting with CO gas, $E_{\text{(CuO-ZnO nanotube)}}$ is the total energy of the CuO-ZnO nanotube structure, and $E_{\text{CO}}$ is the total energy of free CO molecules. The most stable configuration corresponds to a binding energy with the largest negative value.

![Fig. 1](image-url) (A) Four different orientations of CO getting close to four positions to be adsorbed on ZnO nanotube, (B) four different orientations for CuO getting close to four positions to be adsorbed on ZnO nanotube, and (C) three different orientations for CO getting close to CuO-ZnO nanotube.
Charge transfer is calculated from Mulliken charge analysis as follows:

\[ Q_t = Q_{(\text{Adsorbed molecule})} - Q_{(\text{Isolated molecule})} \]  

(3)

In addition, the recovery time of (CO molecules from) ZnO and CuO-ZnO nanotube structures can be obtained as follows [31]:

\[ \tau = \theta_0^{-1} \exp \left( \frac{-E_{\text{ads}}}{kT} \right) \]  

(4)

where \( k \) and \( T \) are the Boltzmann’s constant (8.62 \times 10^{-5} \text{ eV K}^{-1}) and temperature, respectively; \( \theta_0 \) denotes the attempt frequency (\( \theta_0 = 10^{12} \text{s}^{-1} \)).

**Results and discussion**

**CO adsorption on ZnO nanotube**

In this section, the adsorption of CO on ZnO nanotube is investigated. In these calculations, first, the structures of CO and pure ZnO nanotubes were optimized. Then, the C–O bond length in carbon monoxide and Zn–O bond length in ZnO nanotube were calculated as 1.12 and 1.87 Å, respectively. These bond lengths are comparable to those obtained in the previously reported results [32–35].

The binding energies of all 16 configurations of adsorption of CO on ZnO nanotube and C-O bond length (\( d_{C-O} \)) were calculated (Table 1). The calculated binding energies have negative values in all configurations. According to the results, the \( a_3T_2 \) configuration is the most optimal configuration after adsorption. The calculated binding energy at the most optimal position (\( a_3T_2 \)) is equal to −0.63 eV.

This adsorption energy is in accordance with earlier reports about the adsorption of CO/ZnO nanotube [36], H\(_2\) and O\(_2\)/ZnO nanotube [34], and HCHO and O\(_2\)/ZnO nanotube [32]. An et al. [36] studied the adsorption of gas molecules on ZnO (6,0) single-walled nanotubes with and without oxygen vacancy. They showed that CO molecules form C–Zn bonds with a length of 2.67 Å, an adsorption energy of −0.22 eV, and 0.18 \( |e| \) charge transfer from the CO molecules to the nanotube.

The optimal structure is shown in Fig. 2A. The Mulliken charge analysis was used to compute the charge transfer between CO and the surface of ZnO nanotube. The results showed that after the adsorption of CO on ZnO, their charges become more positive and negative, respectively. Thus, during the adsorption process, CO behaves as an electron donor and ZnO as an electron acceptor.

![Fig. 2](image-url)  

(A) Optimized configuration of CO/ZnO nanotube (\( a_3T_2 \)), (B) calculated DOS for ZnO nanotubes (black line), and CO/ZnO nanotube structures for the \( a_3T_2 \) configuration (red line)

| Sites   | \( E_{\text{bind}} \) (eV) | \( d_{C-O} \) (Å) |
|---------|----------------------------|-------------------|
| \( a_1T_1 \) | −0.39                     | 1.11              |
| \( a_1B \)  | −0.58                     | 1.14              |
| \( a_1T_2 \) | −0.37                     | 1.15              |
| \( a_1H \)  | −0.35                     | 1.14              |
| \( a_2T_1 \) | −0.32                     | 1.12              |
| \( a_2B \)  | −0.55                     | 1.16              |
| \( a_2T_2 \) | −0.31                     | 1.11              |
| \( a_2H \)  | −0.33                     | 1.15              |
| \( a_3T_1 \) | −0.46                     | 1.15              |
| \( a_3B \)  | −0.52                     | 1.13              |
| \( a_3T_2 \) | −0.63                     | 1.17              |
| \( a_3H \)  | −0.35                     | 1.14              |
| \( a_4T_1 \) | −0.32                     | 1.11              |
| \( a_4B \)  | −0.36                     | 1.13              |
| \( a_4T_2 \) | −0.33                     | 1.15              |
| \( a_4H \)  | −0.49                     | 1.14              |
of $E_{\text{bind}}$ mean stronger interaction between the CO molecules and ZnO nanotubes, which increases the recovery time.

The energy density of states was calculated before and after the adsorption of CO on ZnO nanotube and the curve is shown in Fig. 2B. No considerable change or evidence of hybridization between the CO molecules and ZnO nanotubes was observed by comparing the density of states of ZnO nanotube with that of CO/ZnO nanotubes near the Fermi level. This result is completely in agreement with the obtained weak adsorption energy and small charge transfer. Therefore, it can be concluded that the electronic properties of the ZnO nanotubes remain unchanged after adsorbing CO molecules.

**Adsorption of CuO on ZnO nanotubes**

Calculations were performed for all possible adsorption configurations. In these calculations, first, the structures of CuO were optimized. Then, the Cu–O bond length in copper oxide was calculated as 1.72 Å which is agreement with other reported Cu–O bond length [37, 38]. The adsorption of CuO molecules on ZnO nanotubes was investigated. The results of adsorption energy of all 16 configurations of CuO molecules on ZnO nanotubes are shown in Table 2.

The results indicate the adsorption of CuO on ZnO nanotube and the formation of CuO-decorated ZnO (CuO-ZnO) nanotube. The configuration of $b_1T_1$ was the most optimal configuration for the CuO-ZnO nanotube as shown in Fig. 3A. In this structure, the bond lengths of O–Zn and Cu–O are 2.32 and 1.70 Å, respectively. The net charge transfer from ZnO nanotube to CuO molecule was calculated as 0.117 electrons.

| Sites | $E_{\text{bind}}$ (eV) | $d_{\text{Cu-O}}$ (Å) |
|-------|-----------------|-----------------|
| $b_1T_1$ | −1.91 | 1.72 |
| $b_1B$ | −1.22 | 1.69 |
| $b_1T_2$ | −0.73 | 1.72 |
| $b_1H$ | −0.84 | 1.72 |
| $b_2T_1$ | −0.87 | 1.68 |
| $b_2B$ | −1.34 | 1.72 |
| $b_2T_2$ | −0.89 | 1.69 |
| $b_2H$ | −0.87 | 1.69 |
| $b_3T_1$ | −0.81 | 1.66 |
| $b_3B$ | −1.21 | 1.69 |
| $b_3T_2$ | −1.57 | 1.77 |
| $b_3H$ | −0.86 | 1.73 |
| $b_4T_1$ | −0.81 | 1.66 |
| $b_4B$ | −1.21 | 1.69 |
| $b_4T_2$ | −0.89 | 1.68 |
| $b_4H$ | −0.91 | 1.72 |

Fig. 3 (A) Optimized configuration of CuO-ZnO nanotube ($b_1T_1$), (B) calculated DOS for ZnO nanotube (black line), and CuO-ZnO nanotube structures for the $b_1T_1$ configuration (green line)

The density of states of ZnO nanotube was calculated before and after adsorbing CuO in the most optimal configuration; the curves relative to Fermi level are plotted in Fig. 3B. As can be observed, the energy density of states for CuO-ZnO nanotube is different from that for ZnO nanotube, particularly around the Fermi level, indicating the proper adsorption of ZnO nanotube. A new peak appears near Fermi level when CuO adsorbed, which suggests the CuO adsorption on ZnO nanotube changes the electronic structure of the ZnO nanotube.

**CO adsorption on CuO-ZnO nanotube**

This section evaluates the mechanism of adsorption of CO on CuO-ZnO nanotube. The adsorption of CO on CuO-ZnO nanotube is investigated for three different configurations of C$_1T$, C$_2T$, and C$_3T$ as shown in Fig. 1C. The binding energies for configurations C$_1T$, C$_2T$, and C$_3T$ are equal to $-4.76$, $-2.86$, and $-1.98$ eV, respectively. Figure 4A illustrates the optimal structure and the bond length for the adsorption of CO on CuO-ZnO nanotube (C$_1T$). The results show that the absorption of CuO on ZnO nanotube enhances the capability of CuO-ZnO nanotube to detect CO gas. The net charge transfer from CO to CuO-ZnO nanotube was computed as 0.3189 electrons.
This result is in agreement with other reported results about the adsorption of O$_2$/Pt-ZnO nanotube [34], O$_2$/Pd-ZnO and HCHO/O$_2$/Pd-ZnO nanotube [32], H$_2$@ZnO-NT:VO [33], CO/Al-ZnO [39], and CO/Al- and Cu–ZnO [40]. Nguyen et al. [39], studied the effect of Al doping on CO adsorption at ZnO(10̅1̅0). They showed that the adsorption energy of CO on Al$_{3c}$-doped ZnO(10̅1̅0) is 1.118 eV and 0.470 electrons to CO charge transfer to the CO molecules. Maarouf et al. [40] investigated the adsorption of CO gas molecule on Cu-doped ZnO nanowires. They found that the adsorption energy of CO on Cu-doped ZnO nanowires is $-1.01 \text{ eV}$ and 0.15 electrons is transferred to the CO molecule.

The recovery time of CuO-ZnO nanotube at room temperature was calculated as $8.63 \times 10^{17}$ s. From the results of recovery time, a larger negative value for $E_{\text{bind}}$ means longer desorption time of CO gas molecules from the CuO-ZnO nanotube. Additionally, the strong adsorption of CO on CuO-ZnO nanotube (i.e., with long recovery time and high adsorption energy) indicates that the CuO-ZnO nanotube slowly recovers to its original state.

Figure 4B shows the changes in the energy density of states of CuO-ZnO nanotube computed after the adsorption of CO gas. The obtained results show the changes in charge distribution in the structure after the adsorption of CO. These changes indicate that the CuO-ZnO nanotube can adsorb CO gas, which is consistent with the results of the adsorption energy.

The electron orbital overlap of bonding atoms is illustrated in Fig. 4C. The obtained results indicate that the orbitals of CO atoms (carbon and oxygen) have a good overlap with the orbital of the oxygen atom in CuO.

According to our calculations, by the adsorption of CuO on ZnO nanotube, the capability of this structure for CO gas detection considerably increases as compared to ZnO nanotube, so this compound can be used in CO gas sensors. Our results are in good agreement with the reported experimental results [41–44]. This experimental studies have demonstrated that the sensing response to CO of the gas sensors using ZnO nanostructures could be enhanced by decorating of CuO.

**Electrical conductivity of optimized configurations**

In this section, the electrical conductivity ($\sigma/\tau$) is calculated as a function of the chemical potential at room temperature (300 K) using Boltzmann Transport Properties (BoltzTrap) code [45]. The variations of electrical conductivity of the ZnO and CuO-ZnO nanotubes were computed before and after the adsorption of CO molecules in the range $-2$ to $2$ eV; the results are illustrated in Fig. 5 (a, b, c, and d). The variations of electrical conductivity in Fig. 5 show that the electrical conductivities of the ZnO and CuO-ZnO nanotubes before and after the adsorption of the CO molecules increase above the Fermi level. Changes in electrical conductivity are related to the changes in the resistivity of the
system, which is a measurable quantity. According to these results, the electrical conductivity in CuO-ZnO nanotube is due to the adsorption of CO by CuO and better electron transfer by ZnO nanotube (according to the energy adsorption calculations).

**Conclusion**

The adsorption of CO gas on CuO-ZnO nanotube was theoretically investigated. The results illustrated that compared to pristine ZnO nanotube, CuO-decorated ZnO nanotube was more sensitive to CO molecules. Moreover, it was found that CO prefers to be adsorbed on CuO-ZnO nanotube with an excellent $E_{\text{bind}}$ of $-4.76$ eV. The density of states revealed the changes in the band gap and charge transfer, which influence the conductivity of the CuO-ZnO nanotube. It was also found that the electrical conductivity of CuO-ZnO nanotube varies in the range $-2$ to $2$ eV. The electrical conductivity of the ZnO and CuO-ZnO nanotube increases above the Fermi surface due to the adsorption of CO on ZnO and CuO-ZnO nanotubes. The results of the binding energy, density of state, and the electrical conductivity of CuO-ZnO nanotube after the adsorption of CO gas imply that the CuO-ZnO nanotube nanostructure can be used to detect CO.

**Author contribution** All authors designed the project; ST and TT did the calculations; all authors contributed to the writing of the manuscript.

**Data availability** N/A.

**Code availability** N/A

**Declarations**

**Ethics approval** This article does not contain any studies with human participants or animals performed by any of the authors.

**Consent to participate** The authors declare the consent to participate.

**Consent for publication** The authors declare the consent for publication.

**Conflict of interest** The authors declare no competing interests.

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