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A theoretical study of ZnO-GS nanosensor to detect H_2S at room temperature

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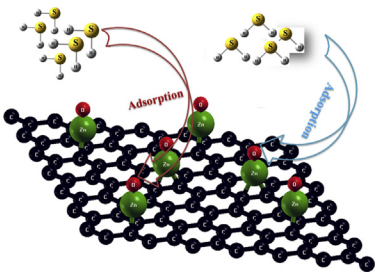
HIGHLIGHTS

- Adsorption mechanism of H_2S on ZnO-GS nanosensors are studied.
- The most stable configuration of each structure is obtained by using DFT method.
- Electrical conductance of ZnO-GS before and after adsorption H_2S are calculated.
- ZnO-GS nanosensor has more sensitivity in H_2S detection.

GRAPHICAL ABSTRACT



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ABSTRACT

In this paper, to detect hydrogen sulfide (H_2S) gas. the electronic structure, density of states, charge population analysis and electrical conductivity change at room temperature for Zinc oxide decorated graphene sheets (ZnO-GS) nanostructure were studied in detail. The calculations were performed using Density Functional Theory. The results strongly showed that the ZnO-GS nanostructure could be used as a nanosensor to detect H_2S gas at room temperature. Based on this set of calculations, H_2S adsorption energy on ZnO-GS showed a significant increase compared to the pure graphene sheets. The electrical conductivity of ZnO-GS was significantly changed at room temperature, after adsorption of H_2S. Based on these studies, the ZnO-GS nanosensor can be used to detect H_2S. Obtained results are in excellent agreement with reported experimental results.

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1. Introduction

Gas sensors have multiple applications including environmental monitoring, safety, medical, military and aerospace activities in human societies. These sensors are of interest to researchers and industry as a result of the volume, sensitivity, and ability to detect gas at low concentrations and low cost. The main characteristics and limits of this technology include measurement ability and duration of gas measurement by the sensor. In recent years, researchers have used nanotechnology to develop a new generation of detectors to eliminate the limitations of sensors, and develop ultra-high sensitivity for gas detection, very fast responsiveness, reversibility, good performance at room temperature, low energy consumption and greater stability. Graphene, as a two-dimensional structure with unique properties, is one of the substances which attracted researchers in the field of nanotechnology.

Zinc oxide (ZnO) is a semiconductor material having a large band gap of about 3.37 eV and binding energy of about 60 MeV at room temperature [1,2]. The ZnO photocatalyst is non-toxic with stable chemical properties and high adsorption rate; on this basis, it

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has been used for various applications such as gas biosensors [3–8]. Given that the energy consumption of sensors made of ZnO nanocrystals is generally high and the sensors work in high temperature, and show relatively poor chemical performance, researchers are trying to produce a material that does not have these weaknesses.

In recent years, the production of nanosensors made by combining graphene with metallic oxides has attracted the interest of researchers. The sensors have high sensitivity at room temperature. So far, the production of nanosensors by combining graphene with metallic oxides such as SnO_2, ZnO, Cu_2O, and WO_3 has been reported [9–18]. Empirical research suggests that the growth of ZnO nanocrystals on graphene sheet is an appropriate sensor to identify compounds like NH_3, CO_2, NO, CO, NO_2 and ethanol in low concentrations (about 1 ppm) [19,20].

In this paper, the structure of the system was simulated for possible modes using density functional theory (DFT), to develop the understanding of the nanosensor of zinc oxide decorated graphene sheets (ZnO-GS), and the adsorption of hydrogen sulfide (H_2S) gas on it was studied. The mechanism of adsorption, electronic structure changes, density of states, charge population analysis and electrical conductivity at room temperature of ZnO-GS nanosensor before and after the adsorption of H_2S gas are the properties studied in this research.

2. Simulation and calculation

In this set of calculations, the atomic geometry and electron structure were determined based on density functional theory (DFT) and by using an extension of the flat wave function and QUANTUM ESPRESSO software [21]. The studied system was chosen to be a graphene supercell with 50 carbon atoms. For the periodic ribbon calculations, a vacuum spacing of 22 Å was introduced along non-repeating directions, and a $8 \times 8 \times 1$ Monkhorst-Pack k-point mesh was used. Marzari-Vanderbilt cold smearing with a width of 0.007 Ry was introduced for improved convergence and for savings in k-point density. To optimize the configurations, exchange-correlation functionals were calculated by generalized gradient approximation (GGA) with PBE function. Further, ultrasoft pseudopotentials and plane-wave cutoffs of wavefunctions of 612 eV along with charge density of 5000 eV were employed. The semi classical of Boltzmann transportation equation is used for calculation of electrical conductance of different configurations at room temperature by Boltzmann Transport Properties (BoltzTrap) code [22]. The input file for this program is results of NSCF calculations with a mesh of $50 \times 50 \times 10$ k-points by QUANTUM ESPRESSO. Finally components of conductance tensor are obtained.

Zinc oxide got close to the graphene sheet in various positions with the symmetry axis parallel and perpendicular to the plane in three states of the carbon-carbon bond bisector perpendicular (Bridge or B-Type), the center of the hexagonal structure of graphene (Hollow or H-Type) and top positions of carbon atoms (Top or T-Type) according to Fig. 1A. Nine possible situations to make ZnO closer to pure graphene sheet with the names of b_1H, b_1B, b_1T, b_2H, b_2B, b_2T, b_3H, b_3B, and b_3T were specified, and the most optimal was selected (Fig. 1B). Then, H_2S gas was made closer to the ZnO-GS nanostructure in three states with the orientation of symmetrical with orientation of hydrogen atoms (C_1(ZnO-GS)), and the hydrogen atom (C_2(ZnO-GS)) and symmetrical with orientation of hydrogen atoms (C_3(ZnO-GS)) and the most optimal state was studied (Fig. 1C). At the end, changes in the electrical conductivity of the ZnO-GS nanostructure at room temperature were calculated to detect H_2S gas.

The binding energy (E_{bind}) of all possible configurations of adsorption of ZnO on GS are calculated by:

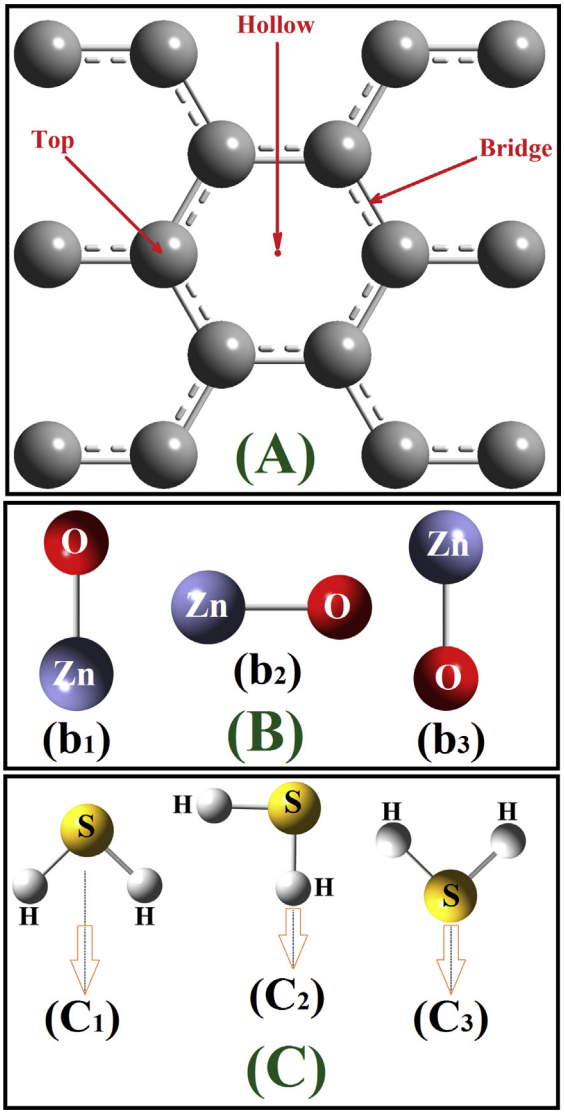

Fig. 1. (A) Schematic view of 3 positions for adsorption of molecule on GS (Hollow (H-Type), Bridge (B-Type) and Top (T-Type)), (B) Schematic view of ZnO interacting with GS in 9 possible adsorption configurations (b_1H, b_1B, b_1T, b_2H, b_2B, b_2T, b_3H, b_3B and b_3T, and (C) Three different orientations for H_2S nearing to ZnO-GS (C_1(ZnO-GS), C_2(ZnO-GS), and C_3(ZnO-GS)).

$$E_{bind} = E_{total} - (E_{GS} + E_{molecule}) \quad (1)$$

where E_{total} is the total energy of the ZnO adsorbed GS, E_{GS} is the total energy of the GS, and $E_{atomormolecule}$ is the total energy of the free ZnO molecule. Moreover, to evaluate the binding energy between the H_2S and ZnO-GS (H_2S/ZnO-GS) structure, E_{bind} is used according to the following equation:

$$E_{bind} = E_{total} - (E_{ZnO-GS} + E_{H_2S}) \quad (2)$$

where the E_{total} is the total energy of the ZnO-GS structure interacting with the H_2S gas. E_{ZnO-GS} is the total energy of the ZnO-GS structure, and E_{H_2S} is the total energy of the free H_2S gas. The most stable configuration happens when binding energy is more negative.

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