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Adsorption study of gas molecules on ZnO decorated carbon nanotubes

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Carbon nanotubes (CNTs) and zinc oxide (ZnO) are one of the most popular materials for gas sensing applications due to its their high electron transfer rate, large specific surface area, promising electronic and structure properties. However, gas sensor based on ZnO nanocluster decorated CNTs is still limited. In this work, we have simulated the models the formation of ZnO nanocluster decorated CNTs and investigated the theoretical study of adsorption of gas molecules (such as methanol, ethanol and isopropanol) on ZnO nanocluster decorated CNTs gas sensor for the first time by using self-consistent charge density functional tight-binding (SCC-DFTB) method. To find the most favorable adsorption configuration, gas molecules were placed at various distances (d) above ZnO surface decorated CNTs. Its interaction energy (⊠E) is calculated by the following equation:
⊠E=E(gas molecules+ZnO-CNTs)-E(ZnO-CNTs)-E(gas molecules), where E(gas molecules+ZnO-CNTs), E(ZnO-CNTs)and E(gas molecules) are the total energies of gas molecules+ZnO-CNTs, ZnO-CNTs and gas molecules systems, respectively. The highest interaction of methanol-ZnO decorated CNTs is found to be -13.28 eV at the distance of 2.60 Å while those of isopropanol-ZnO decorated CNTs and ethanol-ZnO decorated CNTs are -12.75 eV and -12.72 eV at the distance of ˜2.40 Å and ˜2.60 Å, respectively. It can suggest that the ZnO decorated CNTs sensor owns high selectivity to methanol comparising with isopropanol and ethanol. The electronic structures of the ZnO nanocluster decorated CNTs gas sensor before and after gas adsorption will be discussed in more details. The sensing mechanism related to methanol detection will be highlighted.

Keyword: CNTs sensor, ZnO sensor, SCC-DFTB method, ZnO decorated CNT, Gas Sensor, Methanol Sensor

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