COMPUTATIONAL INVESTIGATION ON AN AMIDO-FUNCTIONALIZED SWCNT AS THE SENSING REGION OF A H2S GAS SENSOR

HOSSEINI Kiarash, KALANTARINEZHAD Reza, M.R. SOLEYMANI Yazdi

Iranian University Of Industry and Mine, Tehran, Islamic Republic of Iran

Abstract

Hydrogen sulfide gas is one of the most dangerous gases in oil and gas industry that shall be monitored and detected with high sensitivity and real time detection sensor. During the last decade gas nanosensors based on carbon nanotube and electrical conductance change transduction mechanism have attracted huge attention. Conductometric gas sensors or field effect gas sensors based on one-dimensional nanostructures have been shown to be a promising candidate for enhanced gas sensing, however more investigations are needed to define conductance change mechanisms and important parameters affecting sensor performance. More computational and experimental investigations are needed to elucidate design criteria and understand the effects of different parameters on its performance. In the present work, we are studying the physisorption and the response of the hydrogen sulfide gas sensor. The sensor model comprises an Amido-functionalized semiconducting (8,0) single-walled carbon nanotube interconnected between two gold electrodes on (1,1,1) plane. We investigate the adsorption of a hydrogen sulfide gas on the carbon nanotube channel of a nanosensor using Molecular Dynamics methods and Density Functional Theory in terms of the radial distance of H2S molecules to SWCNT surface and the adsorption energy. Moreover the sensor response is calculated in terms of conductance change calculating electron transport through the device region. The results show that, the carbon nanotube functionalized with amide group responds to H2S gas presence with a conductance change of 1 order of over the linear range.

Keywords: Amide group, SWCNT, DFT (Density Functional Theory), Electro Transport, Molecular Dynamics, Gas sensor, Hydrogen Sulfide (H2S)

Author did not supply full text of the poster.