

Theoretical study of single wall carbon nanotube functionalized with palladium as hydrogen sulfide gas sensorReza Kalantarinejad¹ and Sheida Bagherzadeh Nobari²¹Shezan Company, Iran²Islamic Azad University, Iran

Hydrogen sulfide gas is one of the most dangerous gases for humans because it is toxic, flammable and colorless. In addition to its poisonous characteristics it is mandatory to monitor H₂S in various industries such as coal mining, oil and gas extraction and petrochemical refining. Current commercial sensors work in high temperature and have disadvantages such as high cost and high power consumption. Therefore, it is necessary to develop a fast and safe method to detect H₂S gas in low concentrations with high sensitivity. Field effect gas sensors based on one-dimensional nanostructures have been shown to be a promising candidate for enhanced gas sensing. In this work, the effect of adsorption of H₂S gas on electrical properties of single wall carbon nanotube decorated with palladium nano clusters between two gold electrodes is investigated. For this purpose, current at different bias voltages in absence and presence of H₂S gas was calculated. Then sensitivity of the device at different bias voltages is computed and compared. We find that the largest sensitivity takes place at bias voltage of 40 mV. In this bias voltage, the projected density of states (PDOS) and transmission (T) of SWCNT functionalized with Pd before and after H₂S adsorption are computed and compared accordingly. After adsorption of H₂S gas, the PDOS and as a result T decreased significantly in the energy window between ± 0.02 eV as a result current decreased significantly from 1.53 μ A to 0.89 μ A. This reduction is due to the charge transfer from Pd nano clusters and SWCNT to H₂S gas that results in reduction of concentration of majority carriers (electrons). The results show that carbon nanotube decorated with palladium nanoclusters can be a promising candidate for fabrication of FET gas sensors.

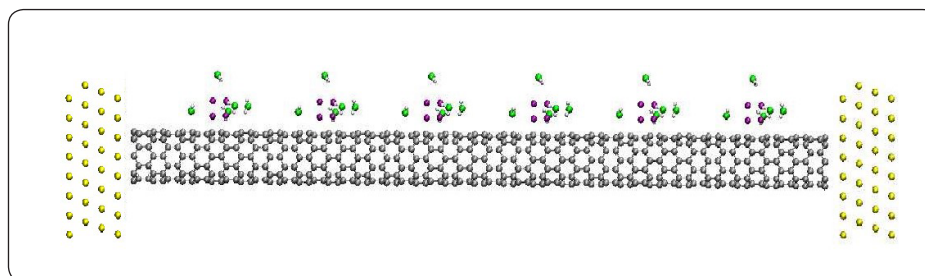


Figure 1: Geometry of the conductometric H₂S sensor based on carbon nanotube decorated with palladium groups. Hydrogen atoms (white), sulfur atoms (green), gold electrodes (yellow), CNT (gray) and palladium clusters (purple).

Recent Publications

1. Bagherzadeh-Nobari S, Hosseini-Istadeh K, Kalantarinejad R, Elahi S M and Shokri A A (2018) Computational investigation of single-wall carbon nanotube functionalized with palladium nanoclusters as hydrogen sulfide gas sensor. *International Nano Letters* 8(1):9-15.
2. Bagherzadeh-Nobari S, Kalantarinejad R, Elahi S M and Sanvito S (2018) Computational investigation of label free detection of biomolecules based on armchair graphene nanoribbon. *Sensors and Actuators B: Chemical* 255:1276-1284.
3. Kalantari-Nejad R, Bahrami M, Rafii-Tabar H, Rungger I and Sanvito S (2010) Computational modeling of a carbon nanotube-based DNA nano sensor. *Nanotechnology* 21(44):445501.
4. Khodadadian A, Hosseini K, Manzour-ol-Ajdad A, Hedayati M, Kalantarinejad R and Heitzinger C (2017) Optimal design of nanowire field-effect troponin sensors. *Computers in Biology and Medicine* 87:46-56.

5. Istadeh K H, Kalantarinejad R, Aghaei M J and Yazdi M R (2013) Computational investigation on H₂S adsorption on the cnt channel of conductometric gas sensor. Journal of Computational and Theoretical Nanoscience 10(11):2708-2713.

Biography

Reza Kalantarinejad has graduated BSc and MSc level in Mechanical Engineering from Amirkabir University of Technology, Tehran, Iran. He conducted his PhD dissertation designing a nano biosensor using modern quantum transport approaches. He has several patents and journal papers in the field of nanotechnology and biotech in particular. He is two-time winner of Kharazmi award and has written over seven books and 20 papers in the field of Nano Biotechnology and Converging Technologies i.e., NBIC (nano, bio, info and cogno techs). He is an entrepreneur in the field of converging technologies and is the founder of Shezan and Hamgara companies; in which he along with his team have successfully developed relevant technological solutions.

kalantari@shezan.com

Notes: