Abstract

Formaldehyde (HCHO) is a massively harmful chemical species whose presence now appears almost in every indoor environment. As people spend most of their time living indoor, be it workplace or home, it is challenging for the occupants to stay away from the exposure of HCHO. The inhalation of gaseous HCHO causes varieties of health complexities, and even the carcinogenic effect of HCHO was identified in the human body. Thus, the onsite detection and monitoring of HCHO vapor have become essential in any confined environment to diminish the potential health hazards. This necessitates the availability of low cost, highly efficient, and miniaturized solid-state HCHO sensors. The present era of intelligent electronics further prefers the sensors to be resistive, for easy integration into the state-of-the-art Complementary Metal Oxide Semiconductor (CMOS) platform to realize the battery-powered and ultra-portable smart detectors. Although the metal oxides (MOX) are the predominant choice as materials for the resistive sensors, their high-temperature operation hosts certain issues like increased power consumption, greater design complexity, reliability problems for the driving circuitry of the sensors, etc. The graphene oxide (GO) is examined in the present dissertation work for the probable low-temperature and low-cost replacement of MOX to address the above-mentioned issues.

The sensitive and selective detection of HCHO molecules at room temperature using the bare GO is challenging. The present research work deals with the theoretical and experimental exploration of different GO derivatives to identify the most appropriate material, which could exhibit the desired sensing performance at room temperature (RT). Density functional theory (DFT) based computational study was employed to observe the changes in energy, structural, and electrical properties (conductivity) of the GO materials upon interaction with HCHO molecules, whereas the experimental data were used to correlate the theoretical outcomes and obtain the practical values of key sensing parameters. At first, the effort was expended to determine the specific functional group of GO having the greatest sensing interaction with HCHO. The graphene oxide containing only those functional groups could be expected to produce improvement in response over the bare GO. The atomic-scale investigation revealed that the graphene oxidized with only hydroxyl (-OH) groups is almost 2 times and 5 times more sensitive than the bare GO and pristine graphene, respectively. However, the response of graphene oxide is still insufficient for real time use, and synthesis of the material is also quite difficult. The functionalization of reduced GO (RGO) with noble metal (Pt, Au, and Ag) nanoparticles was then conducted to get an enhanced sensing performance. Pt functionalized RGO was found to offer the highest response among all the RGO-metal composites. However, the response-recovery of the RGO-Pt was very sluggish, with only partial recovery of the sensor at RT. The hybrid of RGO and SnO_2 was inspected next for complete desorption of molecules at RT and to achieve better response than the RGO-Pt. The experimental data reported that the RGO wrapped SnO_2 exhibits a selective response with magnitude of about 138% (24 times higher than the bare RGO against 200 ppm of HCHO) and response/recovery time of 832 s/765 s at RT. The RGO-SnO_2 composite was found to yield the response characteristics preferred over all the GO derivatives examined in the present thesis work. Thus, the present research work is expected to carry immense significance in paving the way for developing highly efficient and low power RGO based HCHO sensors.

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