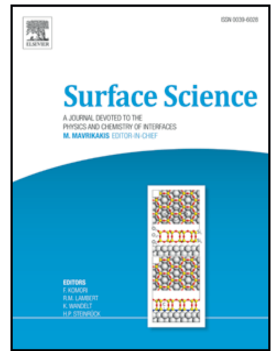
Accepted Manuscript



Cu-, and CuO- decorated graphene as a nanosensor for H2S detection at room temperature

E. Mohammadi-Manesh, M. Vaezzadeh, M. Saeidi

PII: S0039-6028(15)00031-X
DOI: doi: 10.1016/j.susc.2015.02.002
Reference: SUSC 20427

To appear in: *Surface Science*

Received date: 2 November 2014
Accepted date: 4 February 2015

Please cite this article as: E. Mohammadi-Manesh, M. Vaezzadeh, M. Saeidi, Cu-, and CuO- decorated graphene as a nanosensor for H2S detection at room temperature, *Surface Science* (2015), doi: 10.1016/j.susc.2015.02.002

Cu-, and CuO- decorated graphene as a nanosensor for H_2S detection at room temperature

E. Mohammadi-Manesh[a,*], M. Vaezzadeh[a], and M. Saeidi[b]

[a] *Faculty of Physics, K.N.Toosi University of Technology, Tehran, Iran.*
[b] *Department of Physics, Faculty of Basic Sciences, Shahed University, Tehran, Iran.*

Abstract

In this paper, the adsorption mechanism, density of states, charge population analysis and electrical conductance at room temperature are investigated for detection of hydrogen sulfide (H_2S) gas by pure, Cu-, and CuO-decorated graphene sheets (GS). All calculations are done using density functional theory. Results demonstrate that a CuO-GS structure has higher binding energy with H_2S than Cu-GS, and GS. Moreover, the investigated density of states show that orbital hybridization is obviously different between the H_2S and Cu-GS, and the H_2S and CuO-GS, while there is no evidence for hybridization between the H_2S gas and the GS. Furthermore, To find the best nanosensor, electrical conductance of the all possible configurations before and after H_2S adsorption at room temperature is computationally investigated. The obtained results illustrate that electrical conductance of the CuO-GS is significantly changed by H_2S gas adsorption. So, in normal conditions and at room temperatures, the CuO-GS system has more favorable features in detection of H_2S than the GS, and Cu-GS structures.

Keywords: Graphene, Electrical conductance, Hydrogen sulfide, copper oxide, Nanosensor, Density Functional Theory (DFT).

1. Introduction

Fast and exact detection of trace amounts of dangerous gases such as hydrogen sulfide (H_2S) is important in many aspects of human society, i.e. in industrial processes, public health, national security and environmental monitoring. Breathing H_2S is reported to be harmful to human health and can be deadly, depending on the exposure condensation and duration; exposure to only 300 ppm for 30 min is enough to render a worker comatose[1]. It also has damaging effects on many industrial catalysts and is known to be a major source of acid rain when oxidized in the atmosphere. Many industrial processes generate considerable quantities of hydrogen sulfide, including natural gas processing, biogas fermentation, coal gasification, petroleum refining, Kraft mills, and coke ovens. In recent years, interactions of H_2S with semiconductor and metallic surfaces have been investigated computationally and experimentally due to the promising applications of these systems in nanosensor devices[2-15]. The graphene sheet (GS) is considered as an applicable material in production of nanosensors[16,17]. Some experimental researches have shown that the electrical properties of GS can be tuned by doping, and decorating with other atoms, which provide a new route for preparation of good performance graphene based sensing materials. GS has been successfully decorated with numerous atoms and molecules materials including Ag, Au, Cu, CuO, ZnO, Cu_2O salts by different methods [18-25]. Cu and CuO have attracted a great deal of attention because of their various applications. They have been widely used in many important fields such as gas sensors, solar cells, magnetic phase transitions, superconductors and photocatalysts[26-32]. Production methods of Cu-, and CuO- decorated GS (Cu-GS, and CuO-GS) include heating an aqueous solution of Cu salts in the presence of graphene synthesized by an arc discharge method, solvothermal synthesis of CuO-GS and the subsequent reduction of graphene oxide by hydrazine vapor, and chemical reduction of Cu salts in an aqueous solution in the presence of hydrogen induced exfoliated graphene[33-37].

According to the ability of Cu-GS, and CuO-GS production and importance of H_2S detection, a compre-

*Corresponding author.
Email address: emanesh@mail.kntu.ac.ir (E. Mohammadi-Manesh)