

Pre-oxidized Cu₂Si monolayer as toxic gas molecules sensor application

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Abstract

Using first principles calculation, we investigated the adsorption mechanism of small toxic gas molecules (NO, NO₂, NH₃, CO, CO₂, and SO₂) by employing van der Waals (vdW) corrections to study the structural, electronic, magnetic and gas sensing properties of pre-oxidized Cu₂Si monolayer. The sensing mechanism was explored in practical oxygen-rich condition to understand its possibility as a gas sensor. All gas molecules except NO were weakly physisorbed on the pre-oxidized Cu₂Si monolayer, while NO gas molecule shows strong physisorption. It is fascinating to see that all the gas molecules except O₂ act as charge donors, and also adsorption of NO and NO₂ induces small magnetic moments on the non-magnetic pre-oxidized Cu₂Si monolayer. The value of total magnetic moment for NO is 0.56 μ B/cell and for NO₂ is 0.01 μ B/cell, respectively. It is observed that the work function increases by about 2.8% for pre-oxidized condition. Further, the adsorption of gas molecules on the pre-oxidized Cu₂Si monolayer indicates a drop in the work function for NO, CO, CO₂ and rise for NO₂, NH₃, SO₂. Admissible values of adsorption energy assure short recovery time making pre-oxidized Cu₂Si monolayer as an effective nano sensor for harmful toxic gases.

Biography

Yogesh Sonvane is completed Phd at the age of 25 years from Department of Physics, Veer Narmad South Gujarat University (VNSGU), Surat, India in 2011. He is working as Assistant Professor at Applied Physics Department, Sardar Vallabhbhai National Institute of Technology (SVNIT), Surat, India since 2012. He has over 150 publications that have been cited over 200 times, and his/her publication H-index is 15 and has been serving as an editorial board member of reputed Journals.



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