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Absorption of CO_2 on Carbon-based Sensors: First-Principle Analysis. NACIR TIT, Physics Department, UAE University, P.O.Box 15551, Al-Ain, UAE, MOHAMMED ELEZZI, HASAN ABDULLAH, HOCINE BAHLOULI, Physics Department, KFUPM, P.O.Box 1690, Dhahran 31261, Saudi Arabia, ZAIN YAMANI, Center for Research Excellence in Nanotechnology, KFUPM, P.O.Box 5040, Dhahran 31261, Saudi Arabia — We present first-principle investigation of the adsorption properties of CO and CO_2 molecules on both graphene and carbon nanotubes (CNTs) in presence of metal catalysis, mainly iron (Fe). The relaxations were carried out using the self-consistent-charge density-functional tight-binding (SCC-DFTB) code in neglect of heat effects. The results show the following: (1) Defected graphene is found to have high sensitivity and high selectivity towards chemisorption of CO molecules and weak physisorption with CO_2 molecules. (2) In case of CNTs, the iron "Fe" catalyst plays an essential role in capturing CO_2 molecules. The Fe ad-atoms on the surface of CNT introduce huge density of states at Fermi level, but the capture of CO2 molecules would reduce that density and consequently reduce conductivity and increase sensitivity. Concerning the selectivity, we have studied the sensitivity versus various gas molecules (such as: O_2, N_2, H_2, H_2O, and CO). Furthermore, to assess the effect of catalysis on sensitivity, we have studied the sensitivity of other metal catalysts (such as: Ni, Co, Ti, and Sc). We found that CNT-Fe is highly sensitive and selective towards detection of CO and CO_2 molecules. CNT being conductive or semiconducting does not matter much on the adsorption properties.

Nacir Tit
Physics Department, UAE University, P.O.Box 15551

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