First Principle Calculations of the Chemisorption of SO_x on Al-doped Graphene

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Abstract

We have carried out density-functional calculations at the GGA-PBE level to investigate the adsorption of SO, SO_2 and SO_3 on graphene sheets doped with aluminum. We have also compared our results with the zigzag (9,0) and armchair (5,0) carbon nanotubes. We consider here one adsorption configuration in which an Al-S bond is formed. SO adsorbs with adsorption energy − 1.47 eV, and making an Al-S bond of length 2.34 Å. This is comparable to the adsorption energies obtained for adsorption of SO on the nanotubes. For SO_2, the adsorption energy is − 0.65 eV with Al-S bond of length 2.46 Å. The adsorption energy lies between what we got for the Al-doped CNT(9,0) (− 0.76 eV) and the Al-doped CNT(5,5) (− 0.6 eV). For SO_3, the adsorption energy is − 0.85 eV and the Al-S bond length is 2.42 Å. The band gap energy and the charge transferred were found to slightly depend on the adsorbate. SO adsorption does not change the value of the band gap energy, but for SO_2 and SO_3, the band gap energies increase from 0.076 eV to 0.16, and 0.17 eV, respectively. Upon adsorption of the three molecules, the magnitude of the HOMO energy increases by about 0.1, 0.2 and 0.3 eV, respectively, but the increase in the LUMO energy is less. We have also noticed a charge transfer of about −0.2*e*, for SO and SO_2 adsorption, but for SO_3, the charge transferred is about −0.5*e* .

Acknowledgment

This work is funded by King Abdulaziz City for Science and Technology through project no. ART-30-137