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Adsorption of ethanol by using BN nanotube: A DFT study

Maziar Noei[1] , Mojgan Ghaemizadeh[2]

[1] *Department of Chemistry, College of Chemical engineering , Mahshahr Branch, Islamic Azad University, Mahshahr, Iran*

2 Department of Chemistry, College of chemistry, Omidiyeh Branch, Islamic Azad University, Omidiyeh, Iran

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Abstract:

Electrical sensitivity of a boron nitride nanotube (BNNT) was examined toward C_2H_5OH molecules by using density functional theory (DFT) calculations. It was founding that the adsorption energy(E_{ad}) of ethanol on the pristine nanotubes is about -51.5 kJ / mol, but when the nanotube has been doped with Si and Al atoms , the adsorption and recovery time changed and the sensitivity of nanotube toward ethanol was increased. Calculations showed that when the nanotube is doping ,the adsorption energy(E_{ad}) is about -20.2 kJ/mol that leads to decrease the recovery time and also due to doping the nanotube with Si , the amount of HOMO/LUMO energy gap (E_g) will reduce significantly . Therefore, when C_2H_5OH molecule toward to BBNT, the nanotube has produced electrical signals and it seems that these nanotubes can be used as adsorbents for the sensors which are sensitive about C_2H_5OH molecule.

Keywords: Sensor, nanotube, DFT

(*) Corresponding Author: e-mail:maziar.noei@hotmail.com