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Aniline adsorption on the surface of a BN nanotube: Computational study

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Abstract:

Electrical sensitivity of a boron nitride nanotube (BNNT) was examined toward aniline ($C_6H_5NH_2$) molecule by using density functional theory (DFT) calculations at the B3LYP/6-31G (d) level, and it was found that the adsorption energy (E_{ad}) of aniline on the pristine nanotubes is a bout -19.03kcal/mol. But when nanotube has been doped with Si and Al atomes, the adsorption energy of aniline molecule was increase. Calculation showed that when the nanotube is doping by Al, the adsorption energy is about -27.73kcal/mol and also the amount of HOMO/LUMO energy gap (E_g) will reduce significantly. Boron nitride nanotube is a suitable adsorbent for aniline and can be used in separation processes aniline. It is seem that nanotube (BNNT) is a suitable semiconductor after doping, and the doped BNNT in the presence of aniline an electrical signal is generating directly and therefore can potentially be used for aniline sensors.

Keywords: Sensor, Nanotube, DFT, Aniline

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