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Hydroquinone detection by BN nanotube: DFT studies

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Abstract:

Electrical sensitivity of a boron nitride nanotube (BNNT) was examined toward hydroquinone (C6H4(OH)2) molecule by using density functional theory (DFT) calculations at the B3LYP/6-31G(d) level, and it was found that the adsorption energy (Ead) of hydroquinone on the pristine nanotube is a bout -7.77kcal/mol. But when nanotubes have been doped with Si and Al atomes, the adsorption energy of hydroquinone molecule was increased. Calculation showed that when the nanotube is doping by Al, the adsorption energy is about -19.70kcal/mol and also the amount of HOMO/LUMO energy gap (Eg) will reduce significantly. Boron nitride nanotube is a suitable adsorbent for hydroquinone and can be use in separation processes hydroquinone. It is seem that nanotube (BNNT) is a suitable semiconductor after doping, and the doped BNNT in the presence of hydroquinone an electrical signal is generating directly and therefore can potentially be used for hydroquinone sensors.

Keywords, Sensor, Nanotube, DFT, Hydroquinone

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