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C4H6 Adsorption on the Surface of A BN Nanotube: A DFT Studies

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Abstract : Adsorption of a boron nitride nanotube (BNNT) was examined toward ethylacetylene (C4H6) 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 ethylacetylene the pristine nanotubes is about -1.60kcal/mol. But when nanotube have been doped with Si and Al atomes, the adsorption energy of ethylacetylene molecule was increased. Calculation showed that when the nanotube is doping by Al, the adsorption energy is about -24.19kcal/mol and also the amount of HOMO/LUMO energy gap (Eg) will reduce significantly. Boron nitride nanotube is a suitable adsorbent for ethylacetylene and can be used in separation processes ethylacetylene. It is seem that nanotube (BNNT) is a suitable semiconductor after doping, and the doped BNNT in the presence of ethylacetylene an electrical signal is generating directly and therefore can potentially be used for ethylacetylene sensors.

Keywords : sensor, nanotube, DFT, ethylacetylene
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