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Methyl acetylene detection by BN nanotube: DFT studies

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Abstract:

Electrical sensitivity of a boron nitride nanotube (BNNT) was examined toward (C_3H_4) molecule by using density functional theory (DFT) calculations at the B_3LYP/6-31G (d) level, and it was found that the adsorption energy (E_{ad}) of methylacetylene (C_3H_4) the pristine nanotubes is a bout -1.78kcal/mol. But when nanotube have been doped with Si and Al atomes, the adsorption energy of methylacetylene molecule was increased. Calculation showed that when the nanotube is doping by Al, the adsorption energy is about -22.73kcal/mol and also the amount of HOMO/LUMO energy gap (E_g) will reduce significantly. Boron nitride nanotube is a suitable adsorbent for methylacetylene and can be use in separation processes methylacetylene. It is seem that nanotube (BNNT) is a suitable semiconductor after doping, and the doped BNNT in the presence of methylacetylene an electrical signal is generating directly and therefore can potentially be used for methylacetylene sensors.

Keywords, Nanotube, DFT, Methylacetylene,Sensor

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