عنوان مقاله:

Methyl acetylene detection by BN nanotube: DFT studies

محل انتشار:

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خلاصه مقاله:

Electrical sensitivity of a boron nitride nanotube (BNNT) was examined toward (C3H4)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 methylacetylene (C3H4) the pristinenanotubes is a bout -1.78kcal/mol. But when nanotube have been doped with Si and Alatomes, the adsorption energy of methylacetylene molecule was increased. Calculationshowed 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 (Eg) will reducesignificantly. Boron nitride nanotube is a suitable adsorbent for methylacetylene and can beuse in separation processes methylacetylene. It is seem that nanotube (BNNT) is a suitablesemiconductor after doping, and the doped BNNT in the presence of methylacetylene anelectrical signal is generating directly and therefore can potentially be used formethylacetylene sensors.

کلمات کلیدی:

Nanotube, DFT, Methylacetylene,Sensor