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ADSORPTION OF PYRIDINE BY USING BeO NANOTUBE: A DFT STUDY

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Abstract:

Electrical sensitivity of a beryllium oxide nanotube (BeONT) was examined toward (C_5H_5N) molecule by using density functional theory (DFT) calculations at the B3LYP/6-31(d) level, and it was found that the adsorption energy (E_{ad}) of pyridine on the pristine nanotubes is a bout -73.29kcal/mol. But when nanotubes has been doped with S and P atomes , the adsorption energy changed . Calculation showed that when the nanotube is doping by P, the adsorption energy is about -39.59kcal/mol and also the amount of HOMO/LUMO energy gap (E_g) will reduce significantly (Eg=2.55Ev). The BeONT doped with P is suitable semiconductor than the pristine BeONT.

Keywords: Nanotube, DFT, Pyridine

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