



Original Article

## Pyrrole adsorption on the surface of a BN nanotube: A Computational study

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### Abstract:

Electrical sensitivity of a boron nitride nanotube (BNNT) was examined toward pyrrole ( $C_5H_6N$ ) molecule by using density functional theory (DFT) calculations at the B3LYP/6-31G (d) level, and it was found that the adsorption energy ( $E_{ad}$ ) of pyrrole on the pristine nanotubes is about  $-16.37$  kcal/mol. But when nanotube have been doped with Si and Al atoms, the adsorption energy of pyrrole molecule was increased. Calculation showed that when the nanotube is doping by Si, the adsorption energy is about  $-24.29$  kcal/mol and also the amount of HOMO/LUMO energy gap ( $E_g$ ) will reduce significantly. It seems that nanotube (BNNT) is a suitable semiconductor after doping, and the doped BNNT in the presence of pyrrole an electrical signal is generating directly and therefore can potentially be used for pyrrole sensors, and BNNT is a suitable adsorbent for pyrrole molecules.

**Keywords:** Sensor, Nanotube, DFT, Pyrrole

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