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Pyrrole detection by BeO nanotube: DFT studies

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Abstract:

Electrical sensitivity of a beryllium oxide nanotube (BeONT) was examined toward (C₄H₅N) 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 pyrrole on the pristine nanotubes is about -48.58 kcal/mol. But when nanotubes has been doped with S and P atoms, the adsorption energy changed. Calculation showed that when the nanotube is doping by P, the adsorption energy is about -29.04 kcal/mol and also the amount of HOMO/LUMO energy gap (E_g) will reduce significantly. Beryllium oxide nanotube is not suitable adsorbent for pyrrole, but when the BeONT doped by P atom the amount of E_g was less than pristine BeONT and that is a suitable semiconductor.

Keywords, Nanotube, DFT, pyrrole, Sensor
