عنوان مقاله:

Phosphine and Pyrrole detection by using AlN nanotube: DFT studies

محل انتشار:

کنفرانس بین المللی یافته های نوین پژوهشی در شیمی و مهندسی شیمی (سال: 1394)

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خلاصه مقاله:

Electrical sensitivity of an aluminum nitride nanotube (AlNNT) was examined toward pyrrole (C_5H_6N) and phosphine (PH_3) molecules by using density functional theory (DFT) calculations at the B3LYP/6-31G(d) level of theory, and it was found the adsorption energy (E_{ad}) of those molecules on the AlNNT are according to this order: PH_3(E_{ad}=-46.37kcal/mol)> C_5H_6N(E_{ad}=-11.99kcal/mol) when the nanotube have been doped with Si, P, S atoms, the adsorption energy for those molecules on the nanotube were increased. Calculations showed that when the nanotube was doped by those atoms, the amount of HOMO/LUMO energy gap (E_g) reduced significantly. Aluminum nitride nanotube is a suitable adsorbent for detection and separation of those compounds. The result showed that the nanotube (AlNNT) is a suitable semiconductor after doping and the doped AlNNT in the presence of those gases generates an electrical signal and therefore can be used potentially for gas sensors.

کلمات کلیدی:

Sensor, Nanotube, DFT, AlNNT, Pyrrole, Phosphine

لینک ثابت مقاله در پایگاه سیویلیکا:

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