عنوان مقاله:

Investigation of the As, Ga, B and N-doped (6,0) aluminumphosphide nanotubes interactions with H2S gas: DFT study

محل انتشار:

سومین کنفرانس بین المللی دستاوردهای نوین پژوهشی در شیمی و مهندسی شیمی (سال: 1395)

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خلاصه مقاله:

The adsorption behavior of H2S gas molecule on the surface of As, Ga, B and N-doped aluminum phosphide nanotubes are investigated by performing density functional theory calculations. The chemical potential for gas molecule and all studied complexes have been systematically explored. The AIM theory has been also used to examine the properties of the bond critical points: their electron densities andLaplacians. The As-doped nanotube with the adsorption energy of -9.82 kJ/mol has more tendency to the adsorption of H2S gas than the other doped nanotubes. According to the obtained results, the process of H2S molecule adsorption on the surface of As and N-doped AlPNT are exothermic

کلمات کلیدی:

doped-AlPNT, gas adsorption, density functional theory, AIM, HOMO and LUMO

لینک ثابت مقاله در پایگاه سیویلیکا: