عنوان مقاله:

The first principle investigation of adsorption hydrogen cyanide on the surface of Beryllium oxide nanotube

محل انتشار:

سومین همایش ملی تکنولوژی های نوین در شیمی،پتروشیمی و نانو ایران (سال: 1395)

تعداد صفحات اصل مقاله: 5

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خلاصه مقاله:

In this search, the adsorption HCN gas on the outer and inner surface of pristine and Al doped of (4,4) armchair beryllium oxide nanotube are investigated by using DFT theory. For this purpose eight models consider to adsorb of HCN gas at different configuration and all structures optimized, The adsorption energy, Quantum parameters, NMR, DOS and Natural bonding orbitals, and ESP analysis are calculated. The calculated results demonstrate that the adsorption energy HCN gas is negative and all adsorption process is favourable in thermodynamic approach. The .ESP analysis reveals that the density of electron at all models localized near adsorption position

کلمات کلیدی:

BeONTs, DFT, HCN adsorption, Al- doped