عنوان مقاله:

The theoretical study of adsorption of HCN gas on the surface of pristine, Ge, P and GeP-doped (4, 4) armchair BNNTs

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خلاصه مقاله:

In this research, the effects of HCN adsorption on the surface of the pristine, Ge, P, and GeP doped boron nitride nanotube (BNNTs) are investigated by using density function theory at the B3LYP/6–31G(d, p) level of theory. At the first step, we consider different configurations for adsorbing HCN molecule on the surface of BNNTs. The optimized models are used to calculate the structural, electrical, NQR parameters and quantum descriptors such as global hardness, global softness, electrophilicity, gap energy, Fermi level energy, electronic chemical potential, and electronegativity of BNNTs/HCN complex. Inspection of results demonstrates that with doping Ge impurity the sensivity of BNNTs for adsorbing HCN molecule increase significantly from original values. The adsorption of HCN molecule on the surface of Ge-doped is more stable and favourable than other those models. With adsorbing of HCN gas and doping of Ge and GeP the NQR, quantum molecular descriptors and molecular orbital energies of the nanotube alter significantly from original state. On the other hand the electrophilicity index of E model is more than those other models.

کلمات کلیدی:

BNNTs, HCN adsorption, DFT, NQR, DOS