عنوان مقاله:

DFT Investigations for sensing capability of a single-walled Carbon nanotube for adsorptions H۲, N۲, O۲ and CO molecules

محل انتشار:

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خلاصه مقاله:

Single-walled carbon nanotubes (SWCNTs) have a great deal of attention due to their unique properties. These properties of SWCNTs can be used in various devices such as nanosensors. SWCNTs nanosensors have fast response time and high sensitivity to special gas molecules which is very favorable for important applications. Recently, gas adsorption over outer surface of SWCNTs nanosensors was arguably a very interesting theoretical study. Here, the sensing capability of (۶,۰) SWCNTs for adsorption H۲, N۲, O۲ and CO molecules are studied.Thegeometry optimization, electronic, thermodynamic, and vibrational properties have been investigated. All the calculations are based on the density functional theory (DFT) at the B۳LYP/۶-۳۱G level through the Gaussian ۰۹W program package. It is found that, adding these molecules to SWCNT causing a small increase in the bond lengths, and an increase in the total energy. In IR spectra, it is observed increasing the vibration modes and higher stretching vibration wave numbers of SWCNT with the studies molecules. This work confirms that (۶,۰) SWCNT can be used as nanosensor, and using DFT investigations, it is possible to obtain much more data to apply in medical science and industrial technologies.

کلمات کلیدی:

Adsorption energy, DFT, IR spectra, Sensing capability, SWCNT