Study of Sulfur Dioxide Internal and External Adsorption on the Single-Wall Carbon Nanotubes Using Density Functional Theory

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Abstract (Arial 10)
Density-functional theory is used to investigate sulfur dioxide physisorption on inside and outside of single-wall carbon nanotube of (5,0) and (5,5). This study was conducted at B3LYP/6-31G* level of theory. Sulfur dioxide molecule has been studied with axis oriented parallel or perpendicular to the nanotube wall. Both internal and external adsorption on nanotubes increases with the angle of interaction being maximum at 90° to the tube axis. The harmonic frequencies were computed from analytical derivatives for all species in order to define the minimum energy structures. The lowest value of HOMO and LUMO energies is obtained in the process of the adsorption on the external wall of (5,5) nanotube. The dipole moment of the SWCNTs-SO_2 system is highly increased and it is more than SWCNTs- H2S and SWCNTs- CO_2. The lowest ΔG_{tot} for SO_2 on outside wall of (5,0) is obtained while this quantity is positive and not a favorable adsorption process for H2S on the nanotubes. The NBO analysis showed the change in the electronic structure of nanotubes which may be suitable fabricating sensors.

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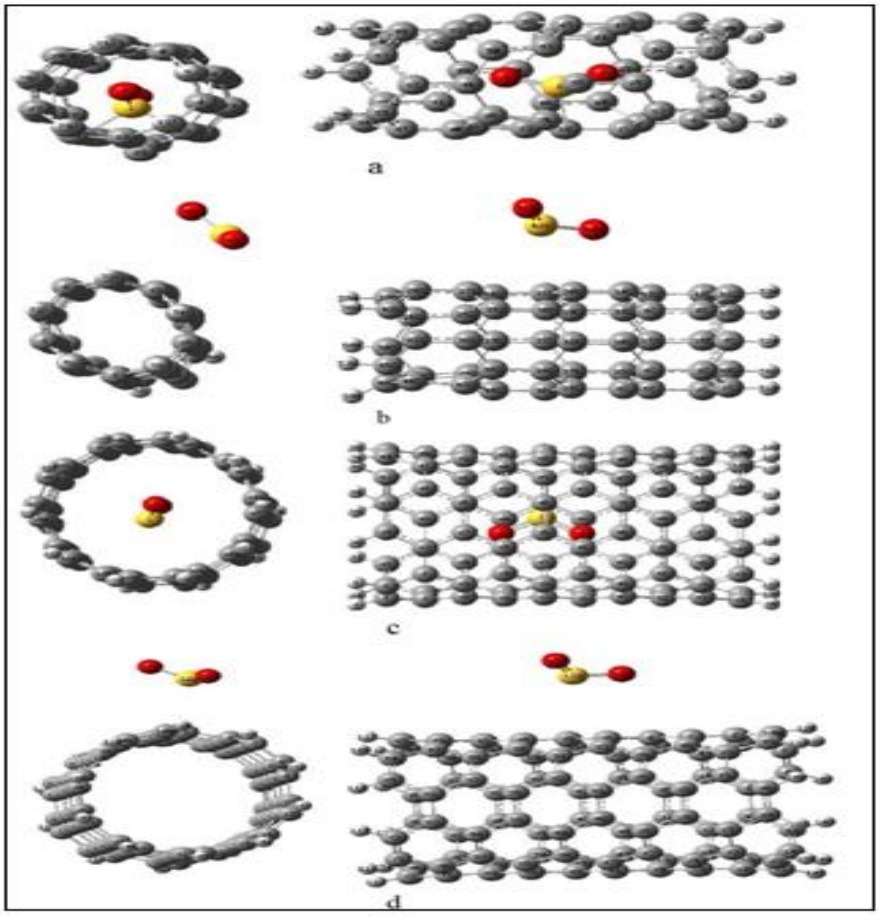

Figure 1 Optimized molecular geometry and interaction between SO2-(5,0) (a, b) and SO2-(5,5) (c, d).

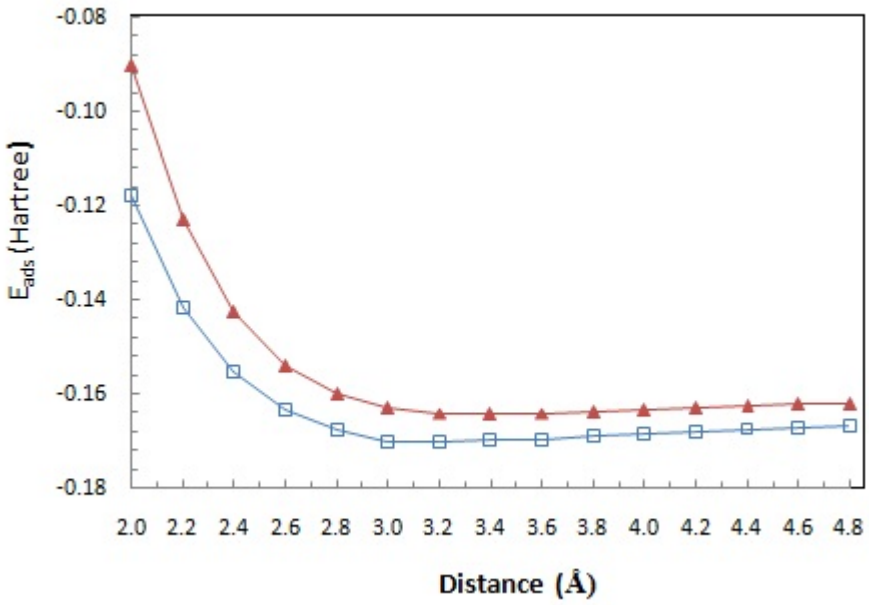

Figure 2 The effect of different distances of SO_2 on external SWCNT, adsorption energy of (5,0) -SO2 (□) and adsorption energy of (5,5) -SO_2 (▲), calculated by B3LYP/6-31G*.