عنوان مقاله:

Investigation of the Interaction of Sulfur Dioxide With Single-Wall Carbon Nanotube of (5,0) by DFT Method

محل انتشار:

اولین همایش نانومواد و نانوتکنولوژی (سال: 1390)

تعداد صفحات اصل مقاله: 11

نویسندگان:

Marzieh Gholamian - *Chemistry Department, Payame Noor University, ۱۹۳۹۵-۴۶۹۷, Tehran, I. R. of Iran*

Mohsen Oftadeh - *Chemistry Department, Payame Noor University, ۱۹۳۹۵-۴۶۹۷, Tehran, I. R. of Iran*

Hassan Hadi Abdallah - *School of Chemical Sciences, Universiti Sains Malaysia, Malaysia*

خلاصه مقاله:

Due to growing increase of pollutants of water and air, some solution should be found to cope with this problem. One of the pollutants is sulfur dioxide, which was investigated in the present study. To study the interaction of sulfur dioxide with inside and outside of zigzag single-wall carbon nanotube of (5,0) were investigated. This study was conducted using DFT at B3LYP/6-31G* level of theory. Computational calculations were performed in the gaseous phase in Gaussian 03. The geometry of all molecules under investigation was determined by optimizing all geometrical variables without any symmetry constraints. The harmonic frequencies were computed from analytical derivatives for all species in order to define the minimum-energy structures. The adsorption energy was calculated through Eads= ENanotube-SO2 – (ENanotube + ESO2) formula. The results showed that thisinteraction on the inside and outside wall of carbon nanotube of (5,0) is maximum at 60 degree vertical to the nanotube main axes. The .thermodynamic properties and charge analysis of the adsorption process were calculated

کلمات کلیدی:

Sulfur dioxide (SO2), Single-wall carbon nanotube (SWCNT), Energy adsorption, Density functional theory (DFT), Sensor