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Computational study of carbon dioxide adsorption on single-walled carbon nanotubes.

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This project deals with the calculation of adsorption energies of carbon dioxide adsorbed on single-walled carbon nanotube with three different radii, namely 1.35, 2.71 and 4.07 Å by using the Density Functional Theory. Our results revealed that carbon dioxide molecule prefers to bind on single-walled carbon nanotubes with the molecular axis parallel to carbon nanotubes surface. Moreover, the adsorption energy of carbon dioxide is inversely proportional to radius of the carbon nanotube. We also found that the distance between center of mass of carbon dioxide molecule and carbon nanotube does not affect to the adsorption energy of carbon dioxide molecule. For charge analysis of carbon dioxide molecule, we found that carbon atom loses two electrons to each oxygen. Consequently, the charge states of carbon and oxygen atoms are +4e and -2e, respectively. Based on the O-C-O angle measurements, we found that the distortion of the carbon dioxide molecule is increased when the radius of carbon nanotube is decreased. This leads to the fact that the reduction of carbon dioxide adsorption energies when the radius of the carbon nanotube is gained comes mainly from the distortion of the carbon dioxide molecule.

Summary

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