

Interaction of adenine and thymine on single-wall carbon nanotubes

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The adsorption of adenine and thymine on the surface of metallic single- wall carbon nanotubes has been studied using local density approximation within density functional theory . After relaxation of the system the energies and equilibrium distances for various configurations which has been reported. To study the adsorption phenomenon of adenine and thymine on SWNT the molecular bonds and angels before and after adsorption were calculated. We studied that all molecules are physisorbed due to the interaction of π -orbitals of adenine-thymine and π - orbitals of SWNT. The study reveals that there is not significant changes due to adsorption in electronic structure of metallic nanotubes. The obtained result from these studies gives insight to investigate the interaction of DNA on surface of single- wall carbon nanotubes.

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