Study of adsorption properties hydroxyurea on carbon and boron nitride nanotubes using density functional theory

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Nanotechnology is a field of practical Knowledge which can cover a wide area. In fact, Nanotechnology is the understanding of the using new properties of materials and systems at the Nanoscale that showing new effects themselves. Recently the use of nanotechnology in medical science is a lot of interest. Nanotube ability for transferring drugs depends on its diameter and the orientation of the incoming molecules. In this study, boron Phosphide, boron nitride, carbon nanotubes, with the Chirality of (7,0), (8,0) and (5,5), respectively, and drug molecule hydroxyurea were drawn through "Nanotube modeler" Software and were optimized by the method of DFT/B3LYP, Basis function 6-31G (d) and using Gaussian software 09. Optimized structures were created by putting the druge molecules on to the nanotubes. Finally, some studies were conducted dipole moment, gap between HOMO and LUMO, ionization potential, hardness, softness, electron affinity and chemical potential of drug molecules before and after placing on to the nanotubes. A number of optimal structures using this method have shown good conductivity and chemical absorption than using Free State of the drugs.

Keywords : Gaussian, Nanotube, Hydroxyurea, Density functional theory.