Study of adsorption properties of procarbazine on the surface of carbon and boron nitride nanotubers using density functional theory.

reza ghoreishi*,

Using different carriers for drug delivery is a fascinating and progressing area in science. Drugs distributd in the body in common fashions like oral and parenteral ways that all parts of body would be influenced by the impact of those and this raise the problem of drug side effects. With the recent development in the modern drug delivery approaches, it would be possible to reach the most efficiency in drug delivery with no damage on other tissues. Therefore, investigation of the properties of drug carriers is of particular importance. With the emergence and development of nanotechnology in the context of drug delivery, it could be possible to utilize nanotubes as the most efficient drug carriers. In the theoretical investigations, drug adsorption on the surface of nanotube is supposed as a first factor in the drug delivery process. So, in this thesis due to the importance of Procarbazine in the cancer treatment, adsorption of that on the surface of carbon and boron nitride nanotubes as drug carriers have been studied. Density functional theory(DFT) and method B3LYP level of theory using 6-31G basis set have been used. In this investigation, binding energy, equilibrium distance, transferred charge, dipole moment, chemical potential, ionization energy, electron affinity and gap of HOMO - LUMO. after adsorption of drug molecule on the surface of nanotube have been calculated. This study shows that some nanotubes have the ability to bind to the drug, and among all, BNNT(5,5) which is dopped with Ga -N site is suggested as the most effective carrier for the transformation of Procarbazine as a drug.

Keywords : Gaussian, anti-cancer drugs, Procarbizine, carbon nanotubes, boron nitride nanotubes, density functional theory