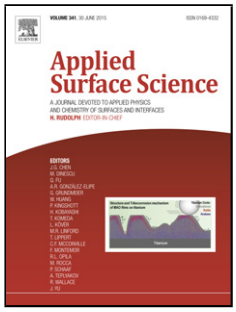

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Investigation of Carboxylation of Carbon Nanotube in the Adsorption of Anti-cancer Drug: A theoretical approach

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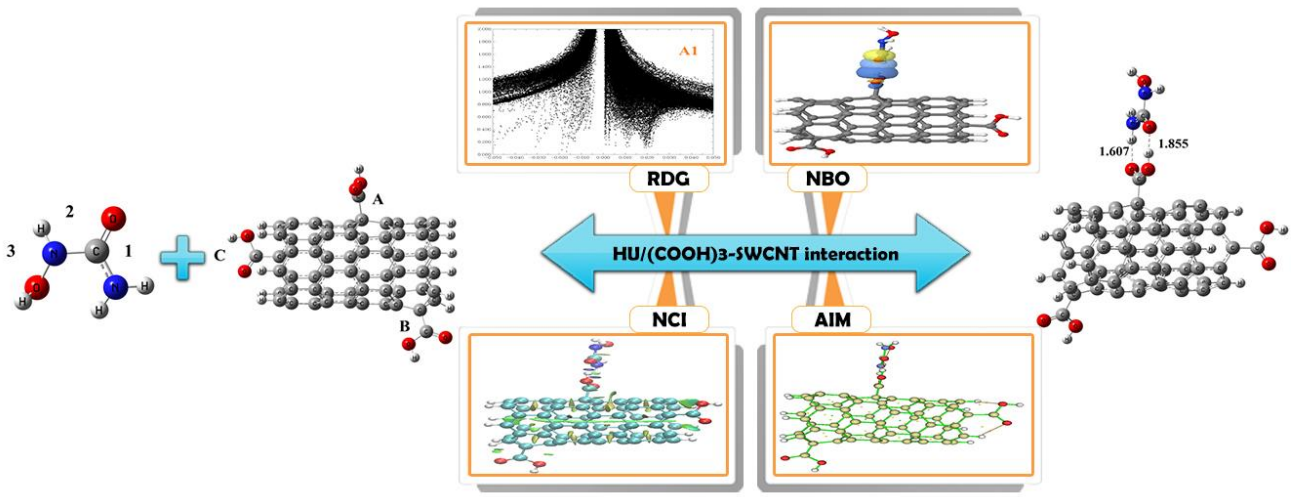
Graphical abstract



HIGHLIGHTS

- Adsorption of anti-cancer drug on carboxylated CNT was studied by DFT method.
- Hydrogen-bonding plays an important role for the stability for complexes.
- NBO, AIM and NCI-RDG analysis confirmed intra-molecular hydrogen bonds between drug and nanotubes.
- The kinetic and thermodynamic parameters indicate that the drug could be adsorbed on the surface of functionalized nanotube better than the pristine nanotube.

ABSTRACT

Nowadays, an important process applied in the design of novel composite materials and drug delivery fields is the carboxylation of carbon nanotubes. In this work, we study the interaction of the anti-cancer drug hydroxyurea with carboxyl-functionalized zigzag carbon nanotubes (CNTs) by employing the method of the density functional theory (DFT) at B3LYP and CAM-B3LYP levels in gas and solvent phases. The results show that all complexes are energetically favorable, especially in the aqueous phase. The enthalpy energy values are negative in all cases, which indicate their exothermic adsorption nature. The presence of –COOH