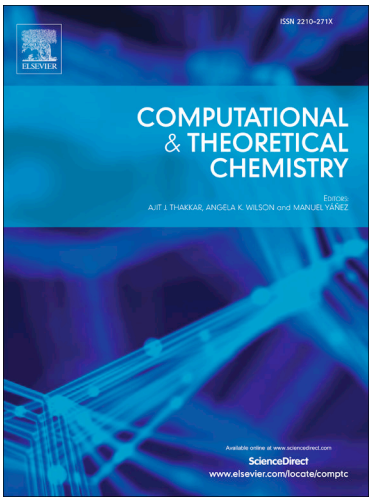

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Interaction between anti-cancer drug hydroxycarbamide and Boron Nitride nanotube: a long-range corrected DFT study

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ABSTRACT

An accurate long-range corrected density functional theory (CAM-B3LYP) is used to optimize hydroxycarbamide (HC) with pristine/Fe-doped boron nitride nanotubes (Fe-BNNTs). In order to investigate the more detailed mechanism of their interactions, Natural Bond Orbital (NBO), Quantum Theory of Atoms in Molecules (QTAIM), and Frontier Molecular Orbital (FMO) calculations are implemented. Weak interactions such as hydrogen bonds and Van der Waals' dispersion are analyzed via the non-covalent interaction index (NCI) as well as the reduced density gradient (RDG) analyses. The molecular electrostatic potential and density of state spectra for all complexes are obtained. The local reactivity of the drug molecule is studied using the Fukui function. Adsorption energies in the gas phase and solution (via IEFPCM model) are also calculated. Based upon the results, all complexes are energetically favorable, especially in the aqueous phase. The calculated results showed that Fe doping in BNNT increases drug-nanotube interaction, especially in case Fe substitutes nitrogen atom.

Keywords: Density Functional Theory; Fe-doped Nanotube; Drug delivery; Non-covalent interaction