A Theoretical Study of Curcumin Adsorption on Linear and Coiled Carbon Nanotubes

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Abstract

Curcumin (CurcH) is a natural compound known as a potent nontoxic, antioxidant, anti-tumor and anti-inflammatory agent with a variety of therapeutic properties such as anti-HIV, anti-bacterial, anticoagulation, antifungal, and antiseptic activities, most interestingly with nontoxic side effects even at high doses. Nevertheless, CurcH suffers from low bio-stability and solubility in the human body during the metabolism process, and also could be affected by some enzyme activities. Therefore, to enhance its solubility and biocompatibility, it is essential to provide the drug with a suitable delivery system. Recently, carbon based nanomaterial has gained a considerable attention leading to a great breakthrough in nanotechnology for its unique physical properties, surface chemistry and structure. Carbon nanotubes (CNTs) are known as superior adsorbents for their unique one dimensional tubular structure, the tendency to establish strong electrostatic π-π interactions and high surface area. In this work, we are interested in a particular structure of these systems: The Coiled Carbon NanoTubes (CCNTs) as innovative delivery systems in attempt to get around the curcumin biodisponibility problems. Our goal is to evaluate the potentialities of using (12,0) zigzag CNT and CCNT as drug nanocarriers systems.
The binding energies for the most stable complexes, electronic properties and nature of interaction were carried out using the Density Functional Tight Binding (DFTB) method. All of the calculations were performed using the program DFTB+.

Keywords: Curcumin, CNT, CCNT, drug delivery, DFTB.