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Theoretical view on interaction between boron nitride nanostructures and some drugs

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ABSTRACT

Many advancing aspects of technology and science are in the field of nanotechnology, in which levels and interfaces are of particular importance in determining the performance and usage. One related application in which interactions play an important role is the synthesis of drugs. Nanotechnology and nanodelivery are comparatively modern procedure and rapidly evolving science that uses nanoscale materials to be used as diagnostic systems or delivery of therapeutic drugs to particular aimed address in a controlled sites manner. Also drug infiltration through cell membranes is a modern challenge. Since Nano boron nitride has unique properties, it is one of the most promising mineral nanostructures ever explored. In this review, all the practical aspects of boron atoms in drug delivery and andnanostructured drugs are surveyed and the nano-boron nitride application is taken in review much more.

1. Introduction

In 2017, a mechanism for drug release based on low pH of cancerous tissues was proposed. According to DFT results, the protons can attack the region of interaction, separating the drug form the carrier. The interaction of 5-FU (5-fluorouracil anti-cancer drug) with pristine fullerene with absorption energy of about -3.2 kcal/mol, which is not suitable for drug delivery, is very poor. To overcome this problem one carbon atom is replaced by a boron atom that increases the adsorption energy to -27.2 kcal per mole. B-doping sensitizes the electronic properties of fullerene to the drug [1] (Figure 1).
Also the electronic sensitivity of the pristine, Al, and Si doped BC_2N nanotubes toward CT drug was studied using DFT calculations. The CT drug prefers to be adsorbed on the all nanotubes via its –NH2 group rather than O-head. The relative reactivity of the studied nanotubes toward the CT drug is as follows: Al-doped » Si-doped > Pristine, with adsorption energy about -48.8, -15.7, and -14.6 kcal/mol (Figure 2).
It was concluded that the Si-doped BC2N nanotube may be a promising candidate for application in CT sensors which benefits form a short recovery time, high sensitivity and selectivity [2].
Due to the rapid development of nanoscience in the production of new drugs, an attempt was made to review the application of boron nitride nanostructures (Figure 3) in the synthesis of effective drugs.

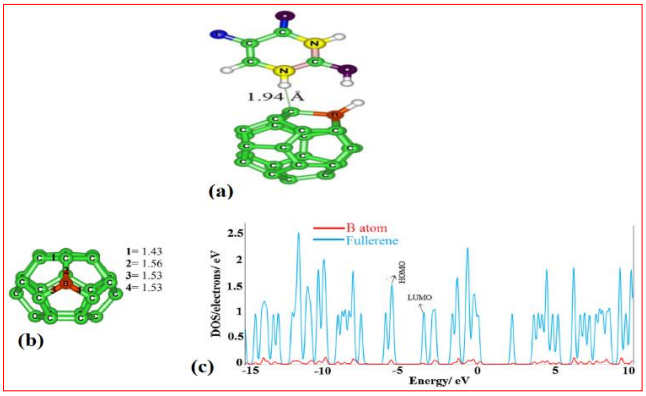

Figure 1. (a) The optimized structure of the 5-FU/B-C24 complex which is assumed to be protonated in the low pH of the cancerous tissues, (b) Optimized structure of B-doped C24 fullerene, (c) Partial density of states (DOS) plot of B-doped C24 fullerene.

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