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# Theoretical investigation of encapsulation of 5-fluorouracil into the BNNTs

Kolsoom Shayan and Alireza Nowroozi*

*Department of Chemistry, Faculty of Science, University of Sistan and Baluchestan (USB), P.O.Box 98135-674, Zahedan, Iran*
**anowroozi@chem.usb.ac.ir*

**ABSTRACT**

*The electronic structure and properties of the armchair boron nitride nanotubes (BNNTs) interacted with the 5-FU drug, as an anticancer drug, are studied at the B3LYP/6-31G(d,p) level of theory. D3-Corrections were carried out for the treatment of intermolecular interactions in the encapsulated nanotubes, exactly. Results have shown that the encapsulation of 5-FU molecule is a favorable process, with a few exceptions. Furthermore, HOMO–LUMO analysis indicated that, after the adsorption process, the HOMO value slightly increased, while the LUMO value in these systems significantly reduced in the Drug@BNNTs complexes. So, the energy gaps between HOMO and LUMO (Eg) are reduced, which emphasis on the greater intermolecular bond strength. The stability and reactivity of the Drug@BNNTs complexes have been examined from the magnitudes of the chemical reactivity descriptors such as chemical potential, global hardness, and electrophilicity index. As a consequence, BNNTs can be considered as a drug delivery vehicle for the transportation of 5-FU as anticancer drug within the biological systems.*

**Keywords: 5-fluorouracil, BNNTs, encapsulated anticancer drugs, HOMO–LUMO analysis**

## 1. INTRODUCTION

Nanomaterials have been investigated in many biological applications, such as drug delivery [1], biosensing [2], and bioimaging [3] due to their novel properties, as well as extreme different functionality, compared to their bulk counterparts. Some of the topologies that have been considered as substrates for these applications include nanotubes (NTs) [2,4], nanowires [5], nanoparticles [6], nanorods [7], and two-dimensional (2D) sheets [8].

Carbon nanotubes (CNTs), one of the fundamental nanomaterials, have been studied for many years in pharmaceutical drug delivery system [9–11]. When CNT is employed as a drug carrier make to happen several biochemical problems about the interactions between drug molecules and carbon nanotube. There are several investigations about this subject experimentally [12,13] and theoretically [14]. The main challenge is low solubility in organic media that can be solved by functionalization for instance with 1,3-dipolar cycloaddition [15] Diels–Alder [16] surfactant molecules [17]. Also, when carbon nanotubes are employed as drug carrier showed low toxicity [18].

Boron nitride nanotubes (BNNTs), one of the emerging nanomaterials, have similar morphology and different properties from CNTs. BNNTs have been considered as capable tool for biomedical adsorption because of