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FeC_{19} cage vehicle for fluorouracil anticancer drug delivery: DFT approach

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ABSTRACT

This work was performed by the importance of applications of nanostructures in drug delivery processes especially for anticancer consumption. Fluorouracil (FU) is a known anticancer drug, in which its loading at the surface of FeC_{19} cage vehicle was investigated by performing density functional theory (DFT) calculations. The employed cage was indeed an iron-doped model of C_{20} cage to provide surface interacting with FU. Seven starting positions (S1 to S7) were predefined for FU to participate in interaction with the cage to provide S1 to S7 complex formations. Optimized structures of six of them were achieved properly, but that of S5 was not achieved even by performing long-hour optimization processes. High strength of obtained complexes approved the complex formation of models and indicating possible role of such metal nanoparticle (MNP) for external filed conducting targeted drug delivery processes. Moreover, the complexes themselves were categorized by the strength level, in which S2 and S4 were introduced as the strongest and the weakest models respectively. Analyses of energies also approved such achievements in addition to confirming results obtained by the atomic scale quadrupole coupling constant (Q_{CC}) parameters. Based on such obtained features of detailed information, FU@FeC_{19} complexes were proposed for drug delivery process.

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1. Introduction

Very soon after the pioneering innovation of carbon nanotube (CNT) in 1991, several attempts have been dedicated to such novel materials regarding their characterizations and further developments [1–3]. Since those early days of CNT innovation, it has been expected that such materials could work unique missions in living systems especially for the cases of drug delivery [4–6]. To this point, considerable efforts have been done to investigate such capability for CNT and other nanomaterials especially for biological systems [7,8]. The results indicated that such expectation could be achieved because of proper surface area of nanostructures for interacting with other substances [9,10]. Furthermore, developments of other nanomaterials indicated that the already known fullerenes could also work very well for such purposes even better than CNT because of their spherical structure [11]. Therefore, attentions have been focused to characterize features of such fullerene based materials in addition to innovating new fullerene-like materials [12–14]. C_{20} is a good example of such fullerene-like martial, which was successfully synthesized and characterized by experiments [15]. The single-standing cage-like small-size C_{20} particle has become topic of numerous research works to initiate new applications based on such unique features of C_{20} cage [16–18]. Regarding chemical aspects, stability of such cage system is very important and then its interaction possibility with other substances is also important to define its chemical reactivity feature for further applications [19]. Moreover, that earlier expectation for application of nanomaterials in living systems has been a leading motor to lead the research topics to such bio-applications of C_{20} [20]. Indeed, carful delivery of drugs avoiding the side effects and keeping the suitable efficacy are both the aims of targeted drug delivery systems, in which the nanomaterials have been always expected to play their dominant role as a vehicle for drugs to carry them up to desired target [21]. The mission is much more important for the cases of those drugs with too many side effects especially in treatments of cancer [22]. In this regard, increasing the efficacy and decreasing the side effects are both two major aims of research works on drug design and delivery for treatments of cancer [23]. Fluorouracil (FU) has been among the most prescribed anticancer drugs for years, but its side effects have always emerged the researchers to improve it for more advantage of consumption for the patients [24–26]. Nanomaterials have been also the topic of such research works on FU to show the advantage of employing such materials for improving the targeted drug delivery features of FU anticancer drug [27–30]. In spite of so many available research results on the topic of developing applications of nanomaterials for FU, the topic is still alive for performing further research works to solve some of unsolved problems in this case [31]. Therefore, investigating applications of nanomaterials for playing vehi-

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