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Two-dimensional silicon carbide monolayer as a promising drug delivery vehicle for hydroxyurea anti-cancer drug

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Abstract−In nanobiotechnology, organic molecule-containing two-dimensional nano-structured materials are considered crucial for developing horizontal bio-inorganic nano-devices for pharmaceutical applications. We present a complete review of the application of silicon carbide monolayer (SiCML) for smart drug delivery of hydroxyurea (HU) through density functional theory computations. Also, interacting host-guest complexes with different approaching orientations, the charge transport, and the interaction strength were scrutinized. It was found that the application of HU together with SiCML was significantly effective for bio-functionalization with −35.86 kcal/mol interaction energy. The charge transfer from HU to the SiCML was confirmed by Hirshfeld method. The findings of the current study provide useful insights into research on the application of functionalized nano-biomaterials for drug delivery, nano-medicine, and other related fields.

Keywords: Silicon Carbide Monolayer, Hydroxyurea, Interaction Energy, Drug Delivery, Nano-biomaterials, Interaction Energy

INTRODUCTION

Improved administration routes of new drugs and a scientific understanding of their delivery are considered important for the safety profile [1-5], since a drug's efficacy is primarily dependent on how it is administered and not on the drug per se [6-11]. Administration of drugs has a significant impact upon their adsorption, medicinal effect period, metabolism, accumulation, related health risks and their pharmacokinetics [12-15]. Drug administration is no simple and easy task. However, one of the novel techniques employed for targeted drug delivery (TDD) is nano-delivery, which is used for improving the biomedical functions of drugs [16,17]. With the bringing of nano-systems into use for TDD, problems such as the degradation of therapeutic agents, solubility issue, high cytotoxicity and lack of specificity at the target site, have been resolved [18, 19]. There have been great advancements in drug delivery and nanotechnology in the last thirty years, which has led to the emergence of nano-medicine as a novel field [20]. Researchers have turned their attention to developing novel drug delivery systems (DDSs) using nano-particles owing to the immensity and versatility of nanotechnology [21-25]. To avoid the side effects of drugs and to improve their selection, researchers have developed various drug delivery mechanisms [26]. In nano-medicine, the main concern is the different properties of drug molecules, such as pharmacokinetics, bio-distribution, cellular absorption, and preferential targeting [27-30].

Estimating drug stabilization, tissue- and cell-controlled targeting and drug release rate is not an easy task. The purpose of drug delivery is to increase the therapeutic efficacy through its in-vivo stabilization, control of its release and the local distribution of the drug [31]. Factors such as the poor solubility of drugs after their administration, safety, and off-target effects hamper the efficacy of many drugs. For instance, unwanted functions might be carried out by most untargeted cardiovascular drugs with toxic compounds, which can cause harmful side effects [32,33]. Engineered nano-materials can be used for improving the pharmacokinetic properties of such drugs. DDSs are conducive to minimizing the adverse effects of different drugs such as cardiovascular drugs [34-38]. To minimize the adverse effects, DDSs distribute the specific drug to the infected or specific location at a predictable rate. One of the prerequisites for a successful TDD is a vector which must be non-toxic and possess acceptable binding abilities. Using nano-carriers with the ability of transporting active ingredients with increased solubility, on-target delivery, and enhanced permeability is the solution to this problem [39-43].

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Nanocarriers are an example of nanotechnology, enjoying the attention of researchers in nano-medicine [44]. In nano-medicine, their pattern is of paramount importance. Researchers and scientists have focused on creating novel and efficient nanocarriers for minimizing the side effects of drugs and enhancing their therapeutic efficacy [45]. The easy off-loading and long-time circulation of nanocarriers is due to their submicron. In preferential drug targeting, it has been proven that two-dimensional nanocarriers such as carbon nano-tubes, graphene (Gr), phosphorene, and fullerenes are efficient [46]. Moreover, researchers have introduced and investigated other two-dimensional structures such as two-dimensional boron nitride (BN), two-dimensional metalorganic frameworks, graphitic carbon nitride (g-C_3N_4), MXenes, layered double hydroxides (LDHs), transition metal oxides (TMOs), black phosphorus (BP) nano-sheets, transition metal dichalcogenides (TMDs) [47-52]. Two-dimensional structures have desirable properties owing to their desirable photothermal effectiveness, ultra-high surface area, biocompatibility, simple functionalization and synthesis, and high stability in physiological environments [53-56]. It is noteworthy that such properties have caused these two-dimensional structures to be considered as promising alternatives in potential biomedical applications such as bioimaging, photothermal therapy, photodynamic therapy, gene delivery, drug delivery, diagnosis, and therapy [57-61]. One of the efforts made in research studies is the search for semi-conducting two-dimensional materials, particularly two-dimensional semiconductors which possess strong in-plane covalent bonds capable of resisting external chemical corrosion and large mechanical deformation. In this regard, the two-dimensional silicon carbide monolayer (SiCML) is considered as a promising candidate not only because of 2.52 eV band gap [62], but also because of its inherited strong structure from Gr. A novel SiCML known as graphene like silicon carbide [63] was recently anticipated by Lu et al., having 1.1 eV band gap and potential optoelectronic applications. As shown in pt-SiC_2 [64] and SiC_3 [65], changing the bonding structure and stoichiometry of two-dimensional SiCMLs might result in significantly different properties based on the review of theoretical advancements in this field. Using particle swarm optimization (PSO), a comprehensive investigation was carried out by Gao, who found that although a cubic SiC_3 structure has exceptional stability at this specific composition, graphite-like SiCMLs are strongly favored [66-68]. Garhpene, with outstanding properties such as the structural stability, high drug loading capacity, and penetrating through the targeted cancerous cell walls, has been utilized in cancer therapy [69]. Another kind of sheet is the boron nitride [70]. The non-toxic and biocompatible properties along with stable binding make BN an efficient candidate as a drug delivery vehicle for cancer treatment [70]. Despite the high potential of the sheets, families in the field of cancer treatment, silicon carbide nanosheet have not been considered as the other members [71]. The most stable silicon carbide can be constructed by SiC sheet, in which the Si to C ratio is 1 : 1 [72]. These structures consist of the alternating C and Si atoms so that each Si atom is surrounded by three C atoms. According to the previous reports, SiC have more advantages compared to graphene. These structures have a reactive exterior surface that facilitates their functionalization in comparison with graphene. Also, the difference between the electronegativities of the Si and C atoms leads to the hydrophilic surface of SiC in contrast to the hydrophobic surface of graphene [73].

Here, we thoroughly investigated the SiCML and the hydroxyurea (HU). Using density functional theory (DFT) calculations, we investigated the interaction between Hu and the SiCML. The structural geometries, the interaction strength, the charge transfers for the interacting host-guest complexes with various approaching configurations were investigated. Furthermore, the electronics structures analysis was accomplished to better understand the interaction nature in the molecule–surface interface. We hope that our theoretical findings will motivate future research works focused on the application of SiC nanostructured biomaterials for developing the relevant biological field of interest.

COMPUTATIONAL DETAILS

We utilized the B3LYP-gCP-D3/6-31G* scheme for carrying out density of states and natural bond orbital analyses along with structural optimizations, energetic and electronic investigations since the functional B3LYP is incapable of predicting dispersion interactions [74-76], and the above-mentioned scheme can modify basis set superposition errors and predict weak interactions effectively [77]. B3LYP has been commonly utilized for investigating the structure of a SiCML [78-83]. Intra- and inter-molecular basis set superposition errors can be predicted through the geometrical counterpoise correction. GAMESS software program was employed for performing all of the computations [84]. We A conductor like polarizable continuum model (CPCM) was adopted for considering the solvation impact [85]. Mulliken charge population analysis and Hirshfeld scheme were employed for evaluating the charge transport between interacting molecular systems [86,87]. The adsorption energy (E_{ad}) was computed as follows:

$$E_{ad} = E_{complex} - (E_{SiC} + E_{drug}) - \delta_{BSSE} \quad (1)$$

where the terms, $E_{complex}$, E_{SiC}, and E_{drug}, respectively, designate the overall energy of the HU/SiC complex, SiCML, and HU. The basis set superposition error (BSSE) correction is designated by δ_{BSSE}, which was computed using the counterpoise method [88].

RESULTS AND DISCUSSION

1. Geometry and Interaction Energy (IE)

First, we scrutinize the interaction of HU with the SiCML surface at solvent (water) media with the B3LYP-gCP-D3 level and 6-31G* basis set to evaluate the interaction of the host-guest system under study. To this end, the relaxed geometry structures of both HU and SiCML (see Fig. 1) have been employed for the interaction process. According to the negatively charged (O/N/C atoms) and positively charged (Si atoms) groups of HU and the SiCML surface, we consider different approaching situations and orientations. Hence, two approaching configurations were considered for the interaction between HU and the surface of the SiCML SiC as shown in Figs. 2(a) and (b), respectively. In configuration A, HU approached the surface of the SiCML so that its -OH and -CO were perpendicular to surface of the monolayer. In configuration B, the -NH_2 and -NH approached the surface of the SiCML in a

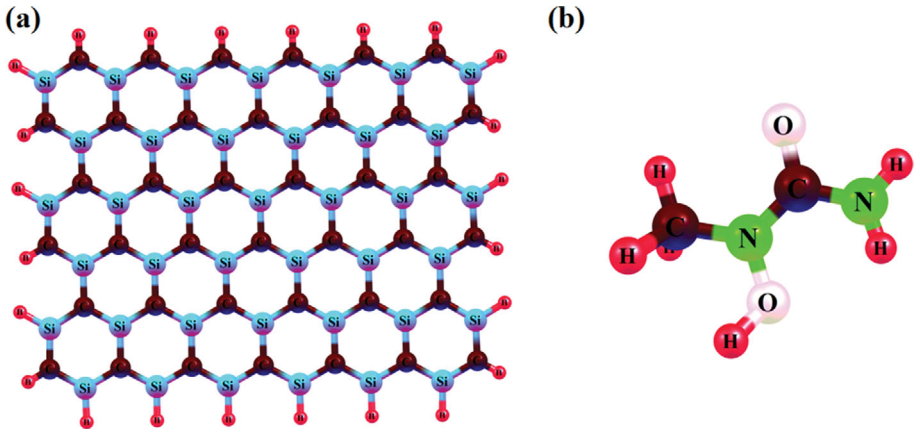

Fig. 1. Optimized geometries of (a) SiCML and (b) HU.

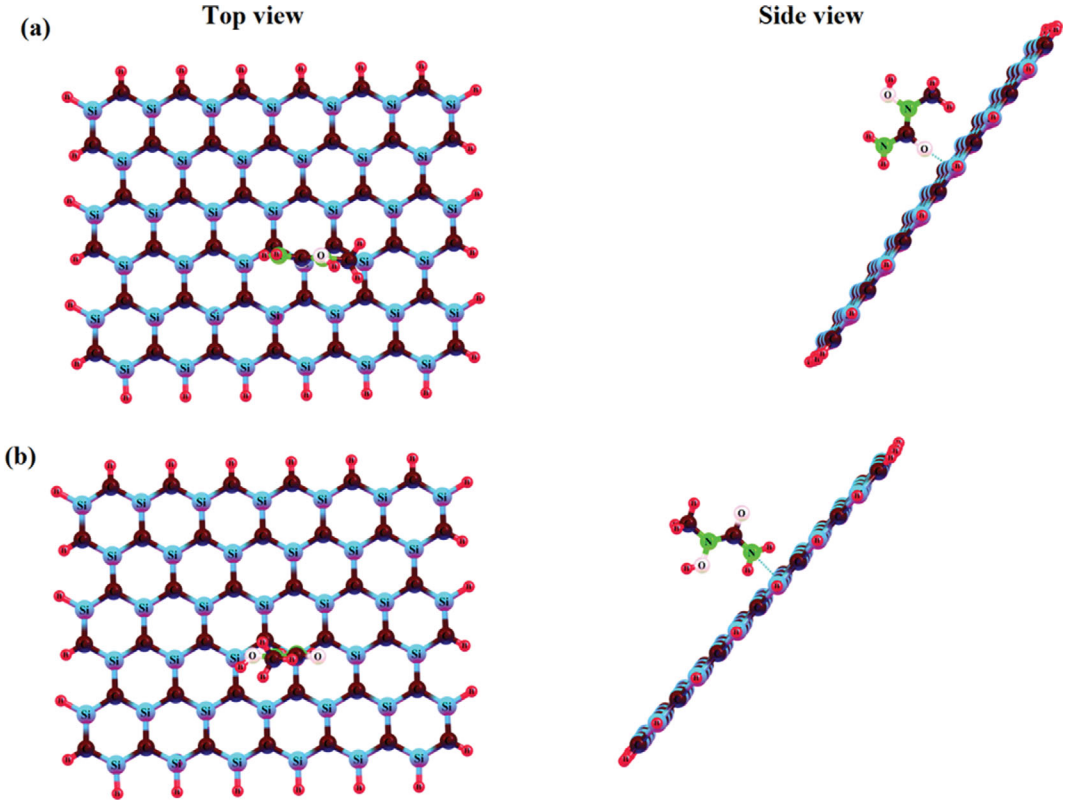

Fig. 2. Optimized configurations (a)-(b) of interactions between SiCML and HU.

way that the Si atoms, as a negatively charged center, approached the Si atoms of SiCML (Fig. 2(b)). Next, we fully relaxed the initial configurations and determined the interaction property. Based on our first-principles computations, in configuration A, HU bounded more strongly to the SiCML than in configuration B. In both configurations, HU oriented towards the surface of the SiCML in a perpendicular fashion. In fact, we positioned the approaching HU in such way that we could improve the dispersion interaction with the surface and reduce the steric hindrance. For the energetically favorable states, we computed adsorption energies to be approximately −35.86 kcal/mol and −15.44 kcal/mol, respectively, for configurations A and B. Relevant vibrational frequencies were computed on final geometries for making sure the optimized geometries have reached the real minimum. Table 1 provides information on interaction energy of optimized HU/SiCML complexes, geometry parameters, and charge transport. Additionally, for the HU/SiCML complex with most stability, the distances between two adjacent atoms (bonding distances) were found to be approximately 1.71 Å. Moreover, relaxed systems' structural geometry parameters demonstrate that the Si-C bond length change marginally from 1.79 to 1.86 Å. Also, the C-O bond length in HU slightly was enlarged from 1.22 to 1.29 Å following the interaction.

Table 1. DFT-computed IE, charge transport, and values of equilibrium distance for HU/SiCML complexes

Systems	E_{ad} (kcal/mol)	d (Å)	Q (e)	ΔG^{o}_{298} (kcal/mol)
Configuration A	−35.86	1.71	0.821	−40.23
Configuration B	−15.44	2.03	0.120	−18.68

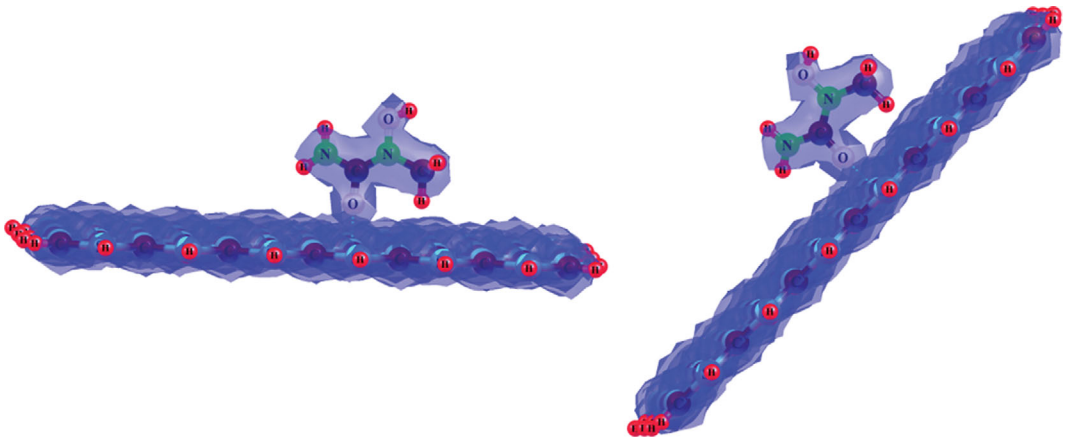

Fig. 3. Schematic diagram of total electron densities of SiCML and HU in configuration A.

According to the literature, a complex formation between corannulene and C_{60} was endergonic (ΔG^{o}_{298}>0) [89]. However, the free energy of the complex of Gr-F4-TCNQ was negative (ΔG^{o}_{298}: −14.5 kcal/mol) [90], which could be ascribed to the strong entropy penalty which is necessary for bringing interacting entities near each other. Thus, from a thermodynamic standpoint, estimating the involved free energy of the reaction is required for assessing the feasibility of the stable complex formation. To do so, the change in the free energy of the reaction was investigated for both configurations of HU/SiCML. We employed the cluster model, including the interaction region, for calculating the free energy for keeping down the computational costs. We computed ΔG^{o}_{298} the structural geometry parameters of to be –40.23 and –18.68 kcal/mol for configurations A and B, respectively. The negative values of free energy demonstrated the thermodynamic feasibility of the complexation of HU with both configurations. However, we found that the stability if configuration A was more at 298 K. The values of adsorption energy indicate that HU presents a strong physisorption process on all of the configurations of nanotube. There are many studies on the interaction of anticancer drugs with the outer surface of different configurations such as nanosheets, nanocage, and nanotubes, which indicate their potential application as drug delivery vehicles [91-93]. For example, the insertion and release of HU on the BN fullerene-like nanocage was investigated by Xu et al. [94]. The E_{ad} of HU on the BN surface is about −17 kJ/mol. In addition, the E_{ad} of HU of the pristine C_{60} was reported to be approximately −6.24 kJ/mol [95], Based on the E_{ad}, the interaction of HU with SiC is stronger than its interaction with the BN nanocage and C_{60}.

For comparison, we estimated interaction energy and carried out the optimization of structural geometry in the gas phase using the same computational procedures for both configurations under study. The interaction energy computed by B3LYP-gCP-D3/6-31G* was observed for the interaction of HU with the SiCML, apart from a negligible change in the adsorption energy of HU. We can see that equilibrium distances were closer to equilibrium distances computed for complexes in the solvent phase. The overall energy of each complex in different media can be subtracted for determining host-guest systems' solvation energy: $E_{solvent}-E_{gas}$. The solvation energy was approximately −5.62 kcal/mol for HU/SiCML complex, showing the potential solvation of the former complex.

2. Charge Transfer Analysis

As it was found from the first-principles calculations, the interaction energy and hence the strength of binding are significantly different and the HU drug prefers to be adsorbed on the SiC surface with configuration A compared to configuration B. The charge populations were analyzed through a valuable Hirshfeld scheme for gaining a deeper understanding into the origins of this difference. Based on out B3LYP-gCP-D3/6-31G* analysis, there was a charge transport of approximately 0.821 e from HU to the SiCML surface in configuration A, while it was 0.12 e in configuration B in the adsorption process. Furthermore, there is a strong interaction between HU and the SiCML based on the charge transfer analysis. Additionally, we computed the total electron density maps to better understand the interacting region of molecular complexes, and Fig. 3 shows the plots. As shown in the density maps, in the interface region of the HU/SiCML system in the interaction region, there is an accumulation of charges. Therefore, the appearance of electron charge density in the interaction region can be the reason for the strong interaction of HU and the SiCML. As the most important quantum chemistry parameters, molecular orbitals such as HOMO and LUMO are considered important in understanding various chemical reactions and reactivity. HOMO is associated with the electron-donating capability of a molecule, and LUMO is associated with its electron-accepting capability. Fig. 4(a) and (b) demonstrate the HOMO and LUMO plots in the most energetically favorable configuration following the adsorption process. We can

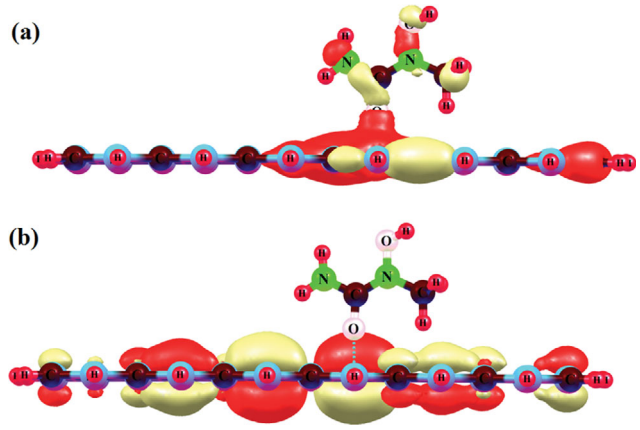

Fig. 4. The calculated orbital localized (a) HOMO (b) LUMO the most stable HU/SiCML complex.

see that the HOMO state is localized on both the SiCML and HU, whereas LUMO state is localized on the SiCML. The evenly distributed HOMO of SiC is greatly redistributed to the side near the adsorption site of HU, thus shifting the HOMO energy of HU@SiC to a higher level. As for the LUMO orbital of HU@SiC, the electron cloud is mainly distributed on HU, which causes the LUMO level to be stabilized. Hence, the redistribution of electron clouds of the HOMO and LUMO of the pristine SiC monolayer results in a decrease in the E_g value for HU@SiC. On the other hand, SiC plays the role of an electron acceptor during the adsorption p, so that it predicts the charge transfer from HU to the SiCML, which is in line with previous claims.

3. Release of Drug

We investigated the process of drug release from the SiCML at the target sites. We demonstrated that the pH of tumor cells is lower than the pH of normal cells. Hence, the influence of pH was evaluated on the most stable structure between HU and the SiCML. The optimized structure of HU/SiCML complexes is represented in an acidic environment (H+species connected to the HU). Moreover, H^+ species should link to the HU's nucleophilic head (O atom). The results demonstrate that, in the acidic environment, the interaction distance between HU and the SiCML increased to 1.71 and 1.94 Å in comparison with the HU/SiCML in the non-acidic environment. Additionally, there was a reduction in E_{ad} in the acidic environment from −35.86 to −30.46 kcal/mol for the HU/SiCML complex, thus leading to weakening of the interaction between HU and the SiCML. Therefore, HU was detached from the carrier while it released into the target sites. The recovery is assessed experimentally by heating the adsorbent to higher temperatures or by exposure to the UV light [96]. The recovery time of nanotubes for the HU desorption can be predicted from the following transition theory:

$$\tau = \upsilon_0^{-1} \exp(-E_{ad}/kT) \quad (2)$$

where ν_0 represents the attempt frequency ($\sim 10^{12}\ s^{-1}$), k is Boltzmann's constant (1.99×10^{-3} kcal $mol^{-1}\cdot K^{-1}$), and T is temperature. The recovery time for HU drug on SiC then will be about 3.62 s at 298 K. These results indicate the SiC suffers from a short recovery time.

CONCLUSION

By using DFT computations, we scrutinized the strong adsorption of HU as a well-known chemotherapy drug in order to produce an original nano-structured material with the capability of interacting with various drugs. We employed SiCML as a promising nano-structure for assessing the impact of polarized Si-C polarized upon the adsorption of and attraction of HU by this unique nano-adsorbent. The interaction energy was computed for scrutinizing the strength of interaction between HU and the SiCML. Based on the B3LYP-gCP-D3/6-31G* computations, HU bonded to the surface of the SiCML via its O atom bonding with the Si atom and the IE was −35.86 kcal/mol and the bonding distance was approximately 1.71 Å, indicating the physisorption nature of the interactions. Based on the charge analysis using the Hirshfeld scheme, there was considerable charge transport between HU and the SiCML (0.821 e). The magnitude of IE and the type of bonding for HU/SiCML complex paves the way for the modeling and development of encouraging SiCMLs for applications in the pharmaceutical industry.

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