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Vitamin-B3 Adsorption by a Ti-Doped Graphene

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Abstract: Vitamin-B3 adsorption with the assistance of titanium (Ti)-doped graphene (TiG) was investigated in this work by performing density functional theory (DFT) calculations. Nicotinic acid (NA) and nicotinamide (NM) were two investigated substances of vitamin B3, which were examined by the adsorption processes towards the TiG surface. Formations of NA...TiG, and NM…TiG complexes were found achievable, and their features indicated the benefits of such complexations for approaching the point of proposing storing containers for the vitamin-B3 substances. Furthermore, the evaluated details of interactions indicated the existence of reasonable strength levels of physical interactions for both NA…TiG, and NM…TiG complexes. Accordingly, the involving molecular sites in interactions indicated a dominant role for the Ti-region in conducting the adsorption process. Additionally, the TiG surface was found as a suitable adsorbent for both substances of vitamin B3. Consequently, the idea of adsorption of vitamin B3 by the employed TiG was affirmed with the results of the current work.

Keywords: vitamin B3; graphene; adsorption; drug delivery; DFT.

1. Introduction

Vitamin B3 is among the required B-type vitamins for maintaining the health quality of human living systems [1]. Nicotinic acid and nicotinamide are two main scaffolds of vitamin B3, in which the ribose group could also be attacked to create a new form of this vitamin as nicotinamide riboside [2]. One major role of indeed all B-type vitamins is energy production through carbohydrates conversion into glucose, besides keeping the health level of different organs such as the liver, skin, and nervous systems [3-5]. Controlling stress-related hormones and inflammations is also found as the function of vitamin B3 [6]. Although a regular diet could supply the required levels of B-type vitamins, their water solubility prevents the body from storing them, and cases of deficiencies could be observed [7-9]. Occurrences of pellagra, sun-sensitive dermatitis, mouth and tongue inflammations, delirium, and even death have been seen as the serious negative impacts of vitamin B3 deficiencies [10]. Accordingly, it is an important issue to make artificial vitamin B3 containers to supply the needs of human body systems [11]. In this regard, the potential of nanostructures for adsorbing other substances could make them suitable for employment in creating vitamin B3 storage containers [12]. Indeed, the surface of nanostructures could be significant in approaching this purpose, and modifying such surfaces

could provide even better tools for adsorbents [13-15]. From the first initiation of nanotechnology, developments of nanostructures for employment in various biomedical applications were considered [16-18].

In the current research work, a representative model of graphene nanostructure was employed for adsorbing two forms of vitamin B3; nicotinic acid and nicotinamide. To this aim, the surface of graphene was modified by an additional titanium (Ti) doping atom to provide a more efficient adsorbent compared with the pure carbon surface. It is worth mentioning that the Ti-related compounds have been found useful for dealing with biological systems; hence, Ti-doped graphene was employed in this work [19]. Quantum chemical calculations were performed to generate the models and their features to approach the goal of proposing efficient adsorbents for the vitamin B3 substances. As shown in Figure 1, singular and bi-molecular models of this work were exhibited, and their features were summarized n Table 1. Indeed, in the case of employing nanostructures for related biological purposes, considerable efforts have been made to this time, but the proposed solutions are not yet certain, and further investigations are still required [20-25]. The terms of initiating drug delivery platforms are among those applications of nanostructures with the highest levels of importance among all other expected applications [26-30]. Accordingly, several attempts have been dedicated to learning the details of such complicated systems of interacting nanostructures and drugs up to now [31-35]. The topic of therapeutic development requires further investigations due to new diseases appearing and remaining unsolved issues of old diseases [36-40]. Hence, the current work could also be related to the drug delivery of vitamin B3 substances for supplying the needs of the human body systems. To approach this point, details of interactions between each of the vitamin B3 substances and the Ti-doped graphene were investigated in the current work to propose a suitable adsorbent surface for storage applications. In this regard, computational chemistry tools were employed to recognize such details to approach the targeted goal of learning the details of adsorption processes and systems [41-45].

2. Materials and Methods

The wB97XD/6-31G* level of density functional theory (DFT) calculations were performed using the Gaussian program [46] to obtain the stabilized geometries of investigated modes of this work. The individual structures of Ti-doped graphene (TiG) and nicotinic acid (NA), and nicotinamide (NM) forms of vitamin B3 and their complexes, including TiG-NA and TiG-NM, are shown in Figure 1. The formulas for TiG, NA, and NM were $C_{40}H_{16}Ti$, $C_6H_5NO_2$, and $C_6H_6N_2O$, in which a Ti atom was inserted among the original carbon atoms of graphene, and the hydrogen atoms terminated the edges to occupy the free valences of carbon atoms. The structures of NA and NM are different in their characteristic functional groups. Based on the structural architecture of NA and NM, two configurations of interactions were found for each of the TiG-NA and TiG-NM complexes. Accordingly, their interactions were revealed by performing additional quantum theory of atoms in molecules (QTAIM) analyses [47,48]. Moreover, frontier molecular orbitals were analyzed for the optimized models, including energy levels of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). To determine energy of adsorption (Ads.), energy differences of complexes and individual substances were compared by considering the impacts of basis set superposition error (BSSE) [49]. The evaluated quantities including interactions types and distances (Int. and Dis.), QTAIM features of the density of all electrons, Laplacian of electron density, and energy density (ρ, $\nabla^2\rho$, and H), HOMO-LUMO energy levels, energy

gap of HOMO and LUMO levels (Gap), and adsorption energy (Ads.) were summarized in Table 1. For visualizing the models and extracting the required information, ChemCraft and MultiWfn programs were used [50,51]. As a consequence, the required information for discussing the models was prepared.

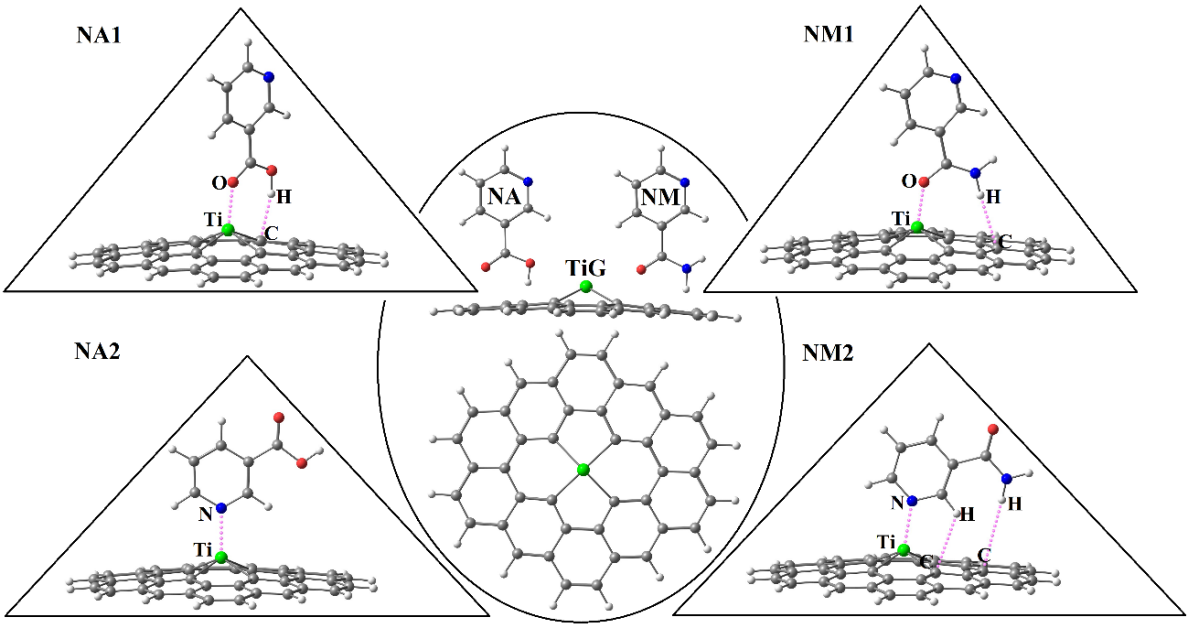

Figure 1. The investigated individual and complex models.

Table 1. Models descriptions.[1]

Description	NA1	NA2	NM1	NM2	TiG	NA	NM
Int.	O…Ti	N…Ti	O…Ti	N…Ti			
Dis. Å	2.065	2.192	2.039	2.191			
ρ au	0.065	0.058	0.069	0.059			
$\nabla^2\rho$ au	0.039	0.271	0.424	0.273			
H au	-0.008	-0.003	-0.007	-0.002			
Int.	H…C		H…C	H…C			
Dis. Å	2.081		2.472	2.809			
ρ au	0.025		0.011	0.008			
$\nabla^2\rho$ au	0.056		0.034	0.024			
H au	-0.002		-0.001	-0.001			
Int.				H…C			
Dis. Å				3.259			
ρ au				0.002			
$\nabla^2\rho$ au				0.008			
H au				-0.001			
Ads. eV	-1.987	-1.975	-2.225	-2.127			
HOMO eV	-6.668	-6.553	-6.548	-6.663	-6.817	-9.419	-9.164
LUMO eV	-1.128	-1.026	-0.891	-0.786	-0.830	0.209	0.534
Gap eV	5.541	5.528	5.657	5.876	5.987	9.627	9.698

[1] The models are exhibited in Figure 1.

3. Results and Discussion

The investigated models of this work are exhibited in Figure 1, and their descriptions are summarized in Table 1. The main difference between NA and NM was their functionalization with a carboxylic group for NA and an amide group for NM, in which their interactions were examined towards the TiG surface to recognize occurrences of NA…TiG and NM…TiG adsorption processes. In these models, two configurations were for each complex system resembling NA1 and NA2 for NA…TiG complexes and NM1 and NM2 for NM…TG

complexes. Differences in configurations were based on the participation of molecular sites of NA and NM towards the TiG surface. As indicated by the optimization calculations, the Ti-region was found as a dominant site of interactions for adsorbing the mentioned NA and NM substances indicating the role of such metal doping in conducting the interaction/adsorption processes. The related descriptions of the optimized models were summarized in Table 1 to describe details of such molecular complexes in the individual and complex states to approach the goal of proposing the employed TiG for storing applications of vitamin-B3 substances.

NA1 and NA2 are two interacting complexes of nicotinic acid and TiG surface, which the results of optimization calculations found them. Based on the results of QTAIM analyses, two interactions were found for NA1; O…Ti and H…C, and one interaction was found for NA2; N…Ti. The results of Table 1 could show higher strength of interactions of NA1 compared to those of NA2, in which the results of adsorption energy are also affirmed by the Ads. values of -1987 eV and -1.975 eV for each of NA1 and NA2, respectively. The H…C interaction of NA1 was a meaningful interaction regarding the obtained QTIAM features, revealing the existence of non-conventional hydrogen bond interactions. Comparing the values of HOMO, LUMO, and Gap of NA1 and NA2 together and with those of the individual TiG and NA, substances could reveal variations of electronic systems for the models before and after complexations. Additionally, the complexes' results were found closer to the individual TiG than the individual NA substance, emphasizing the dominant role of TiG in conducting the adsorption process of NA.

Parallel to the achievements of formations of NA…TiG complexes, two configurations were found for interacting nicotinamide and TiG substances by optimization calculations; NM1 and NM2. The major difference between NA and NM was their functional groups, but a similar route in interactions was observed for both models. As indicated by the exhibited models, NM1 was involved with two interactions; O…Ti and H…C, and NM2 was involved with three interactions; N…Ti, H…C, and H…C. Despite the number of involving interactions, the strength level of O…Ti was found to be higher than that of N…Ti and NM1 were found at a higher level of strength even by comparing the values of Ads.; -2.225 eV for NM1 and -2.127 eV for NM2. Comparing the results with those of NA…TiG complexes indicated a higher level of adsorption strength for NM…TiG complexes. Variations of electronic molecular orbital features indicated a higher similarity of HOMO, LUMO, and Gap of NM1 and NM2 to those of the individual TiG compared with the similarity levels of NA1 and NA2 models.

Based on the obtained results of NA…TiG, and NM…TiG complexes, the models were found suitable for formations, but higher suitability was found for NM…TiG complexes in comparison with the NA…TiG complexes. It should be noted that the models were suitable for formations based on their found configurations, levels of interaction strengths, and adsorption energies. In this regard, an order of NM1 > NM2 > NA1 > NA2 was found to show the adsorption strength. Comparing the results of this work with those of other earlier works on related compounds [12, 52-54] could emphasize the reliability of current results for proposing the successful adsorption of NA and NM substances of vitamin B3 by the TiG surface. Indeed, it was important to find such details of interactions for learning about the adsorption processes of vitamin B3-related substances with the assistance of a representative TiG surface. In this regard, the results affirmed an initial hypothesis of employing the TiG surface for vitamin B3 storage purposes. This could be in two ways of interest: the first way could be for its efficient usage, and the second could be for its long-time storage. Another way of interest could be for separating vitamin-B3 substances from a mixture, in which the employed TiG surface could

work to approach that purpose. Accordingly, it was found that the complex formations of NA…TiG, and NM…TiG models could help to provide a container for the adsorbed substances, in which the strength levels were found in the range of a reasonable physical level of adsorption.

4. Conclusions

Two substances, nicotinic acid (NA) and nicotinamide (NM), of vitamin B3 adsorptions by Ti-doped graphene (TiG) were investigated in this work to approach the goal of proposing a storage container. The models were analyzed, and the results indicated the suitability of the TiG surface for conducting the adsorption process to contain the vitamin B3 substances. Different configurations of relaxations were found for both substances towards the TiG surface with a meaningful level of physical adsorption strengths. The models were recognized by the variations of electronic molecular orbital features assigning a dominant role of TiG for conducting the adsorption processes. In conclusion, the investigated models of NA…TiG, and NM…TiG complexes were found suitable for proposing storing applications of vitamin B3 substances.

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Conflicts of Interest

The authors declare no conflict of interest.

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