

Sensing functions of an iron-doped boron nitride nanocone towards acetaminophen and its thio/thiol analogs: A DFT outlook

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ABSTRACT

Sensing functions of an iron (Fe)-doped boron nitride nanocone (FBN) were investigated towards acetaminophen (ACM) and its thio/thiol analogs by performing density functional theory (DFT) calculations. Formations of FBN-ACM complexes were found through keto/thio and enol/thiol interacting pathways with the Fe-doped region of FBN. The existence of Fe...O, Fe...S, and a type of N...H hydrogen bond interactions were observed in the models. A higher strength of Fe...O in comparison with that of Fe...S was found, in which the keto/thio pathway was found better than the enol/thiol pathway. The estimated duration of recovery time was assessed by the adsorption energies. The conductance was assessed by the energy gaps. Accordingly, meaningful variations of electronic conductance and recovery time were found to provide a suitable situation of sensing function. Consequently, the FBN substance was found as a sensor of ACM and its analogs besides working as an additional proposed role of a drug carrier.

1. Introduction

By the developments of industrial societies, several needs were arisen in accordance with the applications of biological and biomedical related devises and mechanisms [1–4]. In this regard, several applications related to the biological systems were supposed to be initiated to maintain various sides of the life system, in which new technologies and materials were invented to approach the purpose [5–7]. Nanotechnology has been among the most highlighted inventions of recent decades and several efforts have been done to recognize the characteristic features of nanostructures for specifying them into desired applications

up to now [8–10]. Employing the nano-related systems and structures in the biological and living system has been seen among the highlighted expectations from the applications of nanotechnology from its innovation [11–14]. In this regard, single standing nanostructures or their combinations with other functional biological substances were examined to approach insights into developing such biological applications [15–18]. Based on such explorations, developing nano-based drug detection platforms has been a challenging expectation up to now [19–21]. Numerous research works were reported to provide insights into the interactions between drug substances and nanostructures, but the issue has been remained still open for performing further

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investigations [22–25]. It is known that the existences of various types of atomic compositions and structural shapes of nanostructures were recognized in addition to the original carbon nanotubes, in which their specifications and characterizations are still under developments [26–28]. The equality of summation of electronic numbers of boron and nitrogen atoms to that of two carbon atoms made the resulting boron nitride (BN) nanostructure as an appropriate alternative of carbon nanostructures [29]. An activated surface area was provided by the heteroatomic compositions of BN nanostructures for participating in a more efficient interaction pathway with other external molecular and atomic substances [30]. Different electronegativity values of boron and nitrogen atoms made a semi-ionic B–N bond in contrast with the non-ionic C–C bonds of carbon nanostructures. To this point, each of boron and nitrogen atoms of BN nanostructures could work as an independent center for conducting the interactions of surfaces with other substances [31,32]. The results of earlier works indicated benefits of employing BN nanostructures for adsorbing the drug substances towards approaching the drug diagnosis and delivery platforms [33–35]. Additionally, atomistic substitutions of BN nanostructures could lead to generations of modified surfaces with the specified interacting sites for involving in exterior communications [36,37]. Among the atomistic substituents, metal atoms have been seen useful because of providing further vacant orbitals and prospective magnetic features for the modified nanostructure [38–40]. The iron (Fe) atom has been found with a high interest of employing as a substituent of nanostructures [41–43]. Besides its suitable metallic features, Fe is known for the biological systems to be used for the drug delivery platforms [44]. In this regard, the complexes of drug and Fe-doped nanostructures have been extensively investigated up to now to learn details of interactions and adsorption processes [45]. Indeed, participating in adsorption processes has been one of the most important functions of nanostructures since their innovation [46–48]. Within this work, a representative Fe-doped BN nanostructure was assessed towards the detection of acetaminophen drug and its thio/thiol analogs substances. To this aim, density functional theory (DFT) calculations were performed for optimizing the models and evaluating their structural and electronic features by the advantage of employing computational tools for investigating the complicated systems [49–51].

Acetaminophen (Fig. 1) is among analgesics (pain relievers) and antipyretics (fever reducers) drugs for treating fever and pain especially in the cases of colds and sore throats, headaches, toothaches, backaches and muscle aches [52–54]. Besides the suitability of medication by acetaminophen, some types of adverse effects such as liver damages or low efficacy put this drug as a subject of running further investigations in both of structural modifications and combinations [55,56]. The adsorption of acetaminophen with nanostructures has been investigated for approaching two purposes of creating diagnostic systems and conducting drug delivery platforms [57,58]. The existence of acetaminophen in the environmental resources could make it a pollutant of the natural ecosystem, in which its detection and removal should be

considered for saving the health systems [59–61]. It is worth to mention that the developments of biological and biomedical related applications based on the advantages of new materials are essential for enhancing the quality of current life system for approaching various achievements [62–65]. In this regard, this work was performed for assessing the function of a model of Fe-doped BN nanocone (FBN) as a drug detection platform for acetaminophen (ACM). Besides the original keto/enol forms of acetaminophen, thio/thiol analogs (Fig. 1) were also investigated in this work. The FBN model of this work was a conical nanostructure with the composition of boron and nitrogen atoms with one Fe atom at the top apex to provide the interacting site. The obtained features of singular models were exhibited in Fig. 2 and those of the complex models were exhibited in Figs. 3–6. Subsequently, the main goal of this work was investigated by examining formations of FBN-ACM complexes to learn details of interactions and their related features for assessing the investigated FBN adsorbent towards approaching a drug detection platform for ACM. The quantitative results were summarized in Tables 1 and 2.

2. Computational details

Sensing functions of an iron-doped boron nitride nanocone (FBN) as a drug detection platform of acetaminophen (ACM) were investigated in this work by performing density functional theory (DFT) calculations. Besides the original keto/enol form of acetaminophen, thio/thiol forms were also considered in this work by substituting the sulfur atom instead of the original oxygen atoms (Fig. 1). Accordingly, four structures were evaluated for involving in interactions with the FBN adsorbent. The singular models of FBN ($B_{16}FeH_{12}N_{16}$) and ACM ($C_8H_9NO_2$) were optimized first, and their combinations were re-optimized next. The FBN model was composed of boron and nitrogen atoms, in which one iron atom was doped at the apex of conical structure to provide an interaction site for the nanocone towards the ACM substances. The existence of additional hydrogen atoms in the FBN composition was due to avoiding the occurrence of dangling effects of base apex of nanocone. The results of earlier works indicated that considering such transition-metal containing systems could be found suitable for investigating the sensing and adsorbing functions of surfaces towards other substances [66–68]. The performed optimization calculations yielded two minimized configurations of FBN-ACM complexes, in which two heads of ACM were separately involved in interactions with the Fe-doped region of FBN. Subsequently, energies of complexes were calculated and the interactions details were examined by the quantum theory of atoms in molecules (QTAIM) analyses (Table 1 and Fig. 3) [69,70]. It should be noted that the minimized energy levels were examined by performing frequency calculations on the optimized structures to ensure the nonexistence of any imaginary frequency. Additionally, molecular orbitals related descriptors of the highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO) were evaluated for the optimized models in singular and bimolecular states (Table 2). Distribution patterns of HOMO and LUMO were exhibited in Figs. 2 and 4. Moreover, infrared (IR) spectra, density of states (DOS) diagrams, and natural bond orbital (NBO) atomic charges were evaluated for the models (Figs. 2–7). All results of this work were obtained based on the wB97XD DFT functional, the 6-31G* standard basis set for the H, B, C, N, and O atoms, and the LANL2DZ effective core potential (ECP) basis set for the Fe atom using the Gaussian program in a 0 1 charge and multiplicity state [71–74]. For calculating the interaction energies, negligible values of basis set superposition error (BSSE) were found [75]. As a consequence, the FBN-ACM complex models were stabilized and their features were evaluated to reach a point of assessing benefits of employing FBN as a drug detection platform of ACM. The results of IR spectra were visualized by the GaussView program [76], the results of QTAIM were analyzed by the MultiWFN program [77], the results of DOS were visualized by the GaussSum program [78], and other graphical visualizations were done by the ChemCraft program [79]. As the

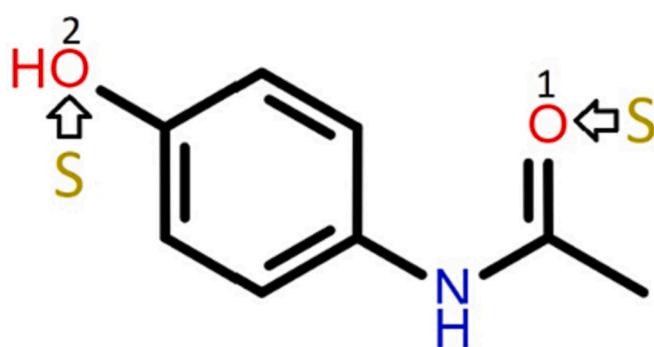


Fig. 1. Acetaminophen (ACM) and thio (1)/thiol (2) substitution places.

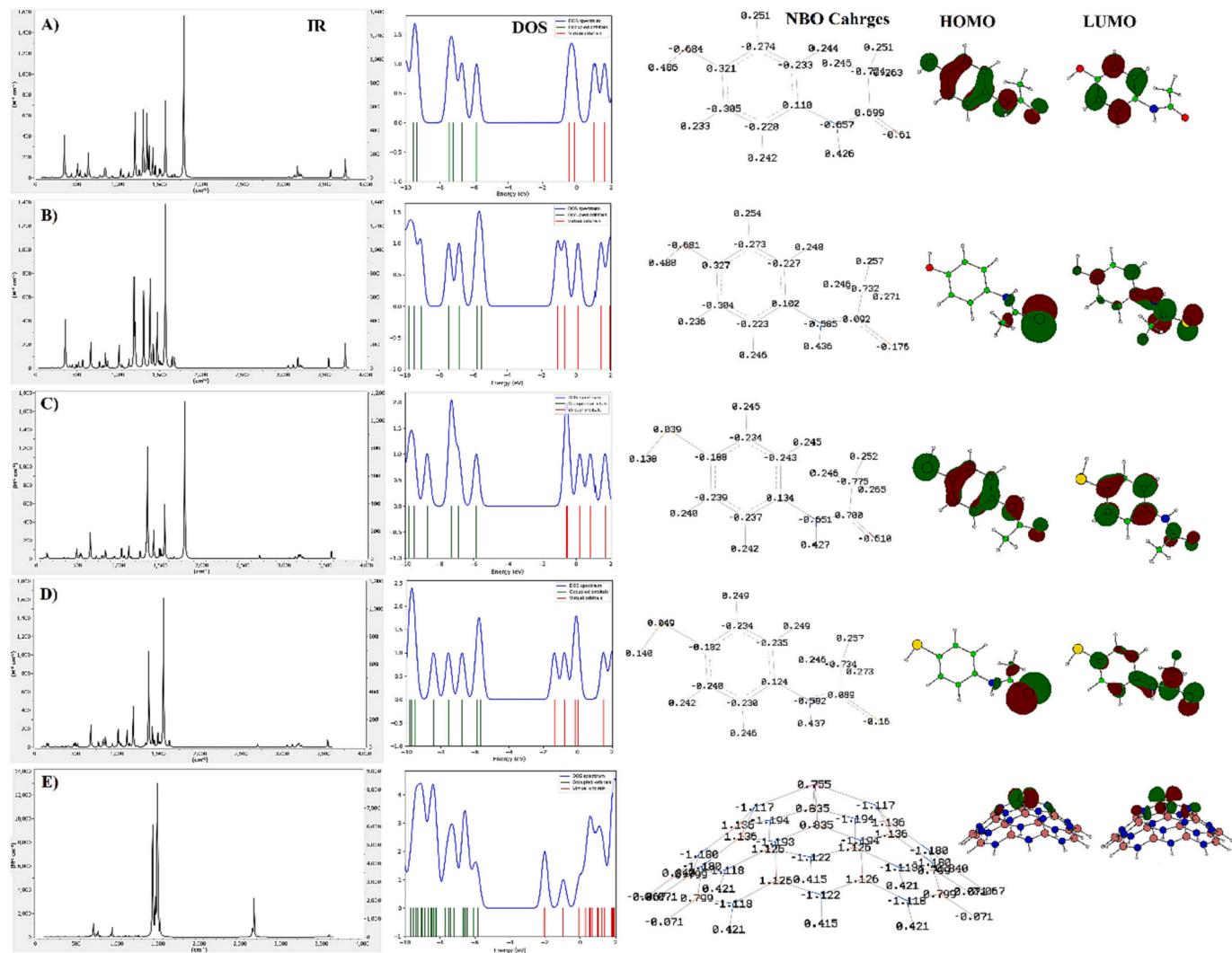


Fig. 2. The evaluated IR spectra (cm^{-1}), DOS diagrams (eV), NBO atomic charges (e), and HOMO-LUMO patterns of singular models: A) the original ACM (O1O2), B) O1-substituted by S (S1O2), C) O2-substituted by S (O1S2), D) O1,O2-substituted by S (S1S2), and E) FBN.

main goal of the current work, the models were analyzed at the smallest molecular and atomic scales using the computational tools for investigating the chemical structures to approach the insights of sensing functions of the FBN substance towards the ACM substances [80,81].

3. Results and discussion

The parental models of this work were a representative model of iron-doped boron nitride nanocone (FBN) and acetaminophen drug (ACM), in which their combinations were investigated to see benefits of initiating a drug detection platform. Indeed, this work was done in accordance with several efforts on developing applications of nano-related materials for working in biological systems media [82–84]. As shown in Fig. 1, ACM has keto (O1) and enol (O2) heads with major capabilities of participating in interactions with other substances. These oxygen atoms were substituted by sulfur atoms to create the thio/thiol forms. The models of ACM were O1O2, S1O2, O1S2, and S1S2, in which their spectral and electronic futures were exhibited in Fig. 2. The features of FBN model were also exhibited in Fig. 2. One Fe atom was doped at the top apex of BN nanocone to create the FBN adsorbent for examining the adsorptions of ACM analogs. The interacting ACM and FBN (FBN-ACM) complexes were exhibited in Fig. 3 along with their NBO atomic charges in Fig. 4.

For optimizing the complex models, adsorptions of both 1 and 2 sides

of ACM were investigated towards the Fe-doped region of FBN. Accordingly, eight models were obtained as shown in panels A-H of Fig. 3. The keto/thio head of ACM participated in interactions with the Fe-doped region of FBN in configurations A, C, E, and G; the enol/thiol head of ACM participated in interactions with the Fe-doped region of FBN in configurations B, D, F, and H. It should be mentioned that the obtained configurations were at the highest feasibility of formations and they were converged in the optimization calculations. Accordingly, the direction of interactions between ACM and FBN was through the keto/thio and enol/thiol heads of ACM to the Fe-doped region of FBN. Two interactions were observed between the substances including $\text{Fe}\cdots\text{O}$, $\text{Fe}\cdots\text{S}$ and $\text{N}\cdots\text{H}$ interactions in each of the FBN-ACM models, in which they were recognized by performing the QTAIM analyses. As listed in Table 1, details of interactions were found and their strengths were recognized. Interactions (Int.), distances (Dis.), total electron density (ρ), Laplacian of electron density ($\nabla^2\rho$), energy density (H), and molecular interaction energy (E_{Int}) were extracted for learning details of interacting FBN-ACM complexes. To evaluate the values of E_{Int} , the energies of complex and singular models were compared by including BSSE through Eq. (1). Other values; Int., Dis., ρ , $\nabla^2\rho$, H, were directly extracted from the output files.

$$E_{\text{Int}} = E_{\text{FBN-ACM}} - E_{\text{FBN}} - E_{\text{ACM}} + \text{BSSE} \quad (1)$$

By the last descriptor of Table 1 (E_{Int}), the formations of

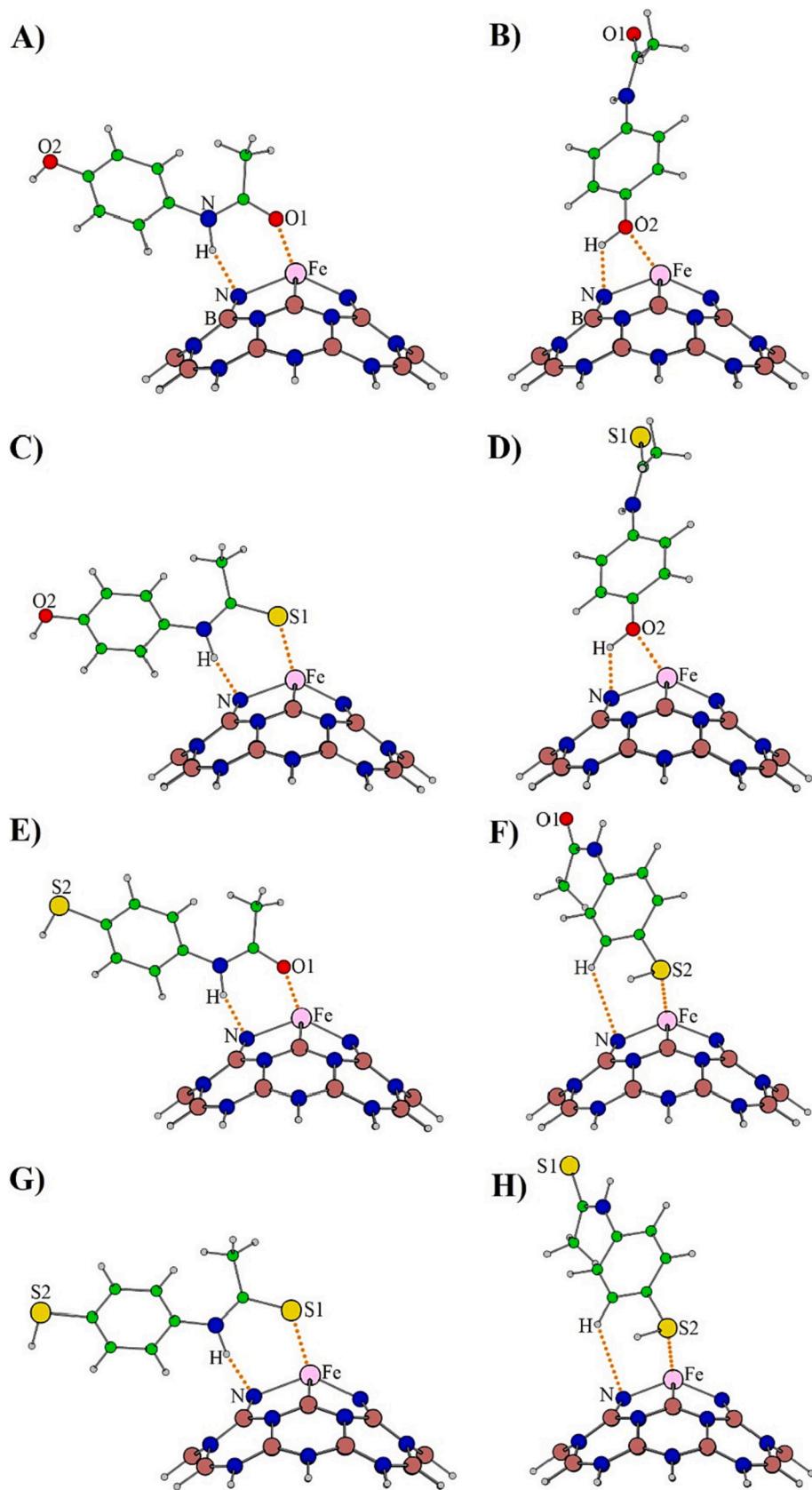


Fig. 3. The obtained configurations of FBN-ACM complexes.

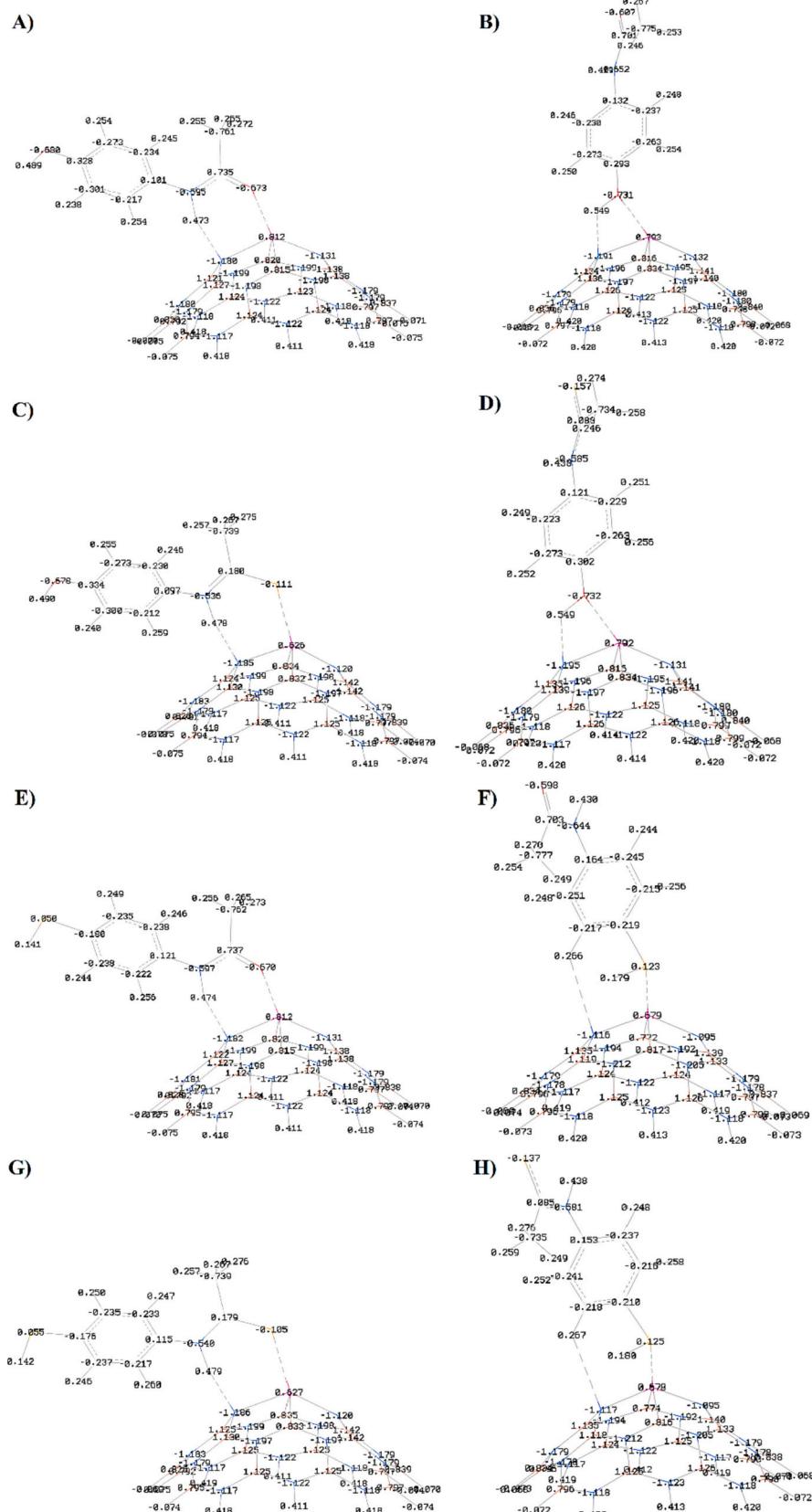


Fig. 4. The obtained NBO atomic charges (e) of FBN-ACM complexes.

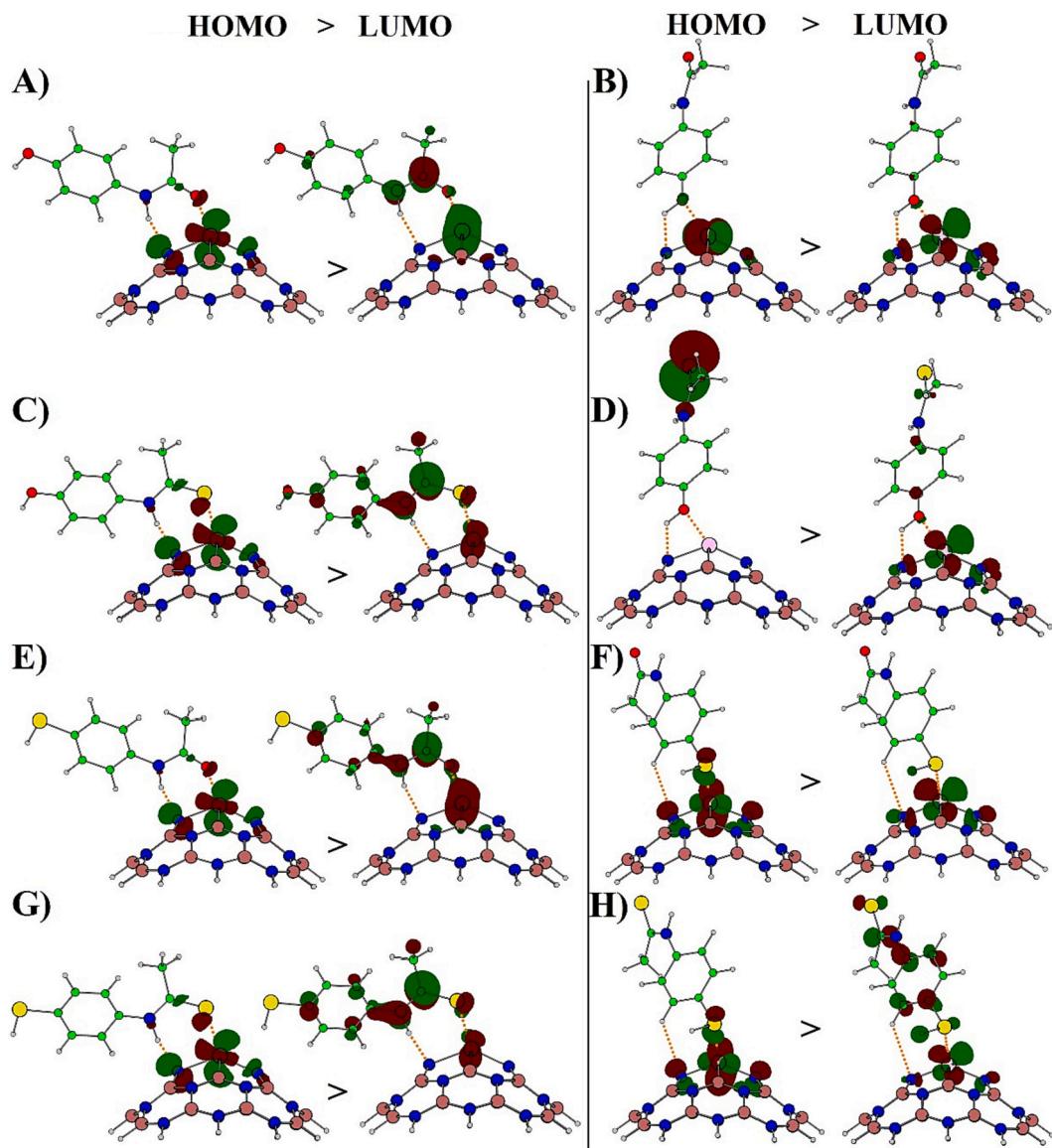


Fig. 5. HOMO and LUMO distribution patterns of two configurations of FBN-ACM complexes.

configurations were categorized based on the strength of interactions between FBN and ACM substances. Configurations A and E were found at the highest level of strength and configurations F and H were found at the lowest level of strength. An obtained achievement is that the formation of Fe...O interaction was more suitable than the formation of Fe...S interaction. Additionally, the keto/thio head (O1 or S1) was at a higher level of favorability of participating in interactions in comparison with the enol/thiol head (O2 or S2). Accordingly, O1O2 and O1S2 models were found at the highest suitability of adsorptions because of formations of Fe...O1 interactions whereas O1S2 and S1S2 were at the lowest suitability of adsorptions because of formations of Fe...S2 interactions. In this regard, it could be assumed that the models were in different models of complex strengths because of their values of interactions energies. Additionally, one N...H interaction was found in all the complexes between the nitrogen atom of FBN and the hydrogen atoms of ACM models. However, that hydrogen atom was different in the models (Fig. 2); it was an amine hydrogen in A, C, E, and G configurations but it was an enol hydrogen in B and D configurations and it was a hydrophobic hydrogen in F and H configurations. It was a benefit of employing the heteroatomic FBN adsorbent for providing an atomic site of involving N...H interactions as a possible type of hydrogen bond

even with a hydrophobic hydrogen atom of ACM.

To show the features of atoms of the models, the evaluated NBO atomic charges were shown in Fig. 4. The results indicated variations of atomic charges among the investigated models, which could be a reason of formation of different strengths of interactions between each of the FBN and ACM complexes. The Fe atom had indeed a leading role for managing the interaction process, and it detected different electronic environment among the FBN-ACM complexes. As a consequence, the models were found in different levels of interactions strengths. Comparing the charges of singular and complex models could show various situations of electron sharing among the interacting substances of complexes to show changes of the models interactions strengths. It is important to mention here that the evaluated NBO atomic charges could help to recognize the suitability of size of employed nanocone for examining the adsorption processes of ACM substances. Comparing the results of those B and N atoms of bottom-edges of FBN nanocone model in the singular and complex states could show that the changes of atomic charges were almost negligible. Additionally, the relaxed configuration of ACM towards the FBN model was almost at the Fe-doped region showing the dominant role of top-apex of the nanocone for participating in interactions with the ACM substance. In this regard, the investigated

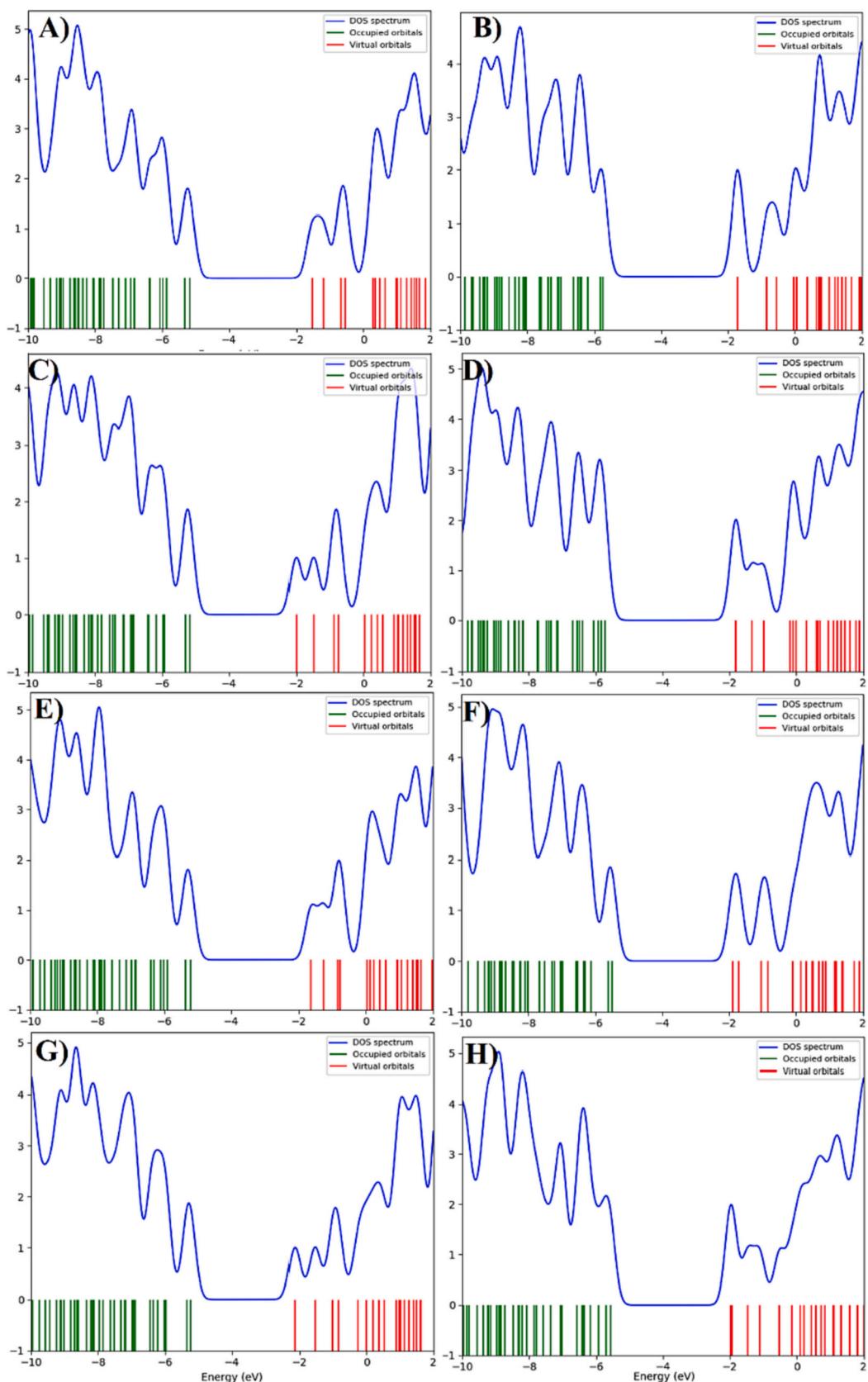


Fig. 6. DOS diagrams of FBN-ACM complexes.

Table 1Interactions details of FBN-ACM complexes.^a

FBN-PCM	Int.	Dis. Å	ρ au	$\nabla^2\rho$ au	H au	E_{int} kcal/mol
A	Fe...O1	1.931	0.088	0.512	-0.065	-30.714
	N...H	1.777	0.045	0.114	-0.036	
B	Fe...O2	2.024	0.066	0.406	-0.049	-18.566
	N...H	1.762	0.047	0.137	-0.039	
C	Fe...S1	2.305	0.073	0.137	-0.024	-24.101
	N...H	1.739	0.049	0.118	-0.005	
D	Fe...O2	2.031	0.064	0.394	-0.048	-17.991
	N...H	1.727	0.051	0.142	-0.004	
E	Fe...O1	1.934	0.087	0.506	-0.049	-30.193
	N...H	1.767	0.046	0.116	-0.038	
F	Fe...S2	2.488	0.051	0.104	-0.015	-10.452
	N...H	2.817	0.007	0.021	0.007	
G	Fe...S1	2.308	0.073	0.136	-0.025	-23.712
	N...H	1.732	0.051	0.119	-0.004	
H	Fe...S2	2.497	0.051	0.103	-0.015	-9.728
	N...H	2.828	0.006	0.019	0.001	

^a The models were shown in Fig. 3.**Table 2**Frontier molecular orbitals details of ACM, FBN, and FBN-ACM models.^a

Model	HOMO eV	LUMO eV	GAP eV	Fermi eV
O1O2	-5.848	-0.423	5.425	-3.136
S1O2	-5.523	-1.062	4.462	-3.293
O1S2	-5.842	-0.573	5.269	-3.207
S1S2	-5.665	-1.334	4.331	-3.499
FBN	-5.838	-2.019	3.818	-3.929
A	-5.156	-1.534	3.622	-3.345
B	-5.748	-1.712	4.036	-3.730
C	-5.169	-2.008	3.161	-3.589
D	-5.729	-1.827	3.902	-3.778
E	-5.216	-1.640	3.576	-3.428
F	-5.489	-1.891	3.598	-3.690
G	-5.224	-2.134	3.090	-3.679
H	-5.564	-1.989	3.574	-3.777

^a The models were shown in Figs. 2 and 3.

size of FBN model was suitable for investigating the purpose in addition to the main goal of this work to perform calculations at the smallest molecular and atomic scales of pure ACM and FBN substances to learn their own natures of interaction participations for the FBN-ACM complex formations.

To better show the electronic features of the investigated models, HOMO and LUMO distribution patterns were exhibited in Figs. 2 and 5 for the singular and complex models. As described above, the models of interacting FBN-ACM complexes were found in two keto/thio (O1/S1) and enol/thiol (O2/S2) interactions pathways of ACM with the FBN substance. The results of Fig. 4 indicated different NBO atomic charges and the results of Figs. 2 and 5 indicated different situations of HOMO and LUMO distribution patterns. Accordingly, the models were recognized based on their electronic situations regarding their frontier molecular orbitals features. Additionally, the evaluated magnitudes of energy levels for HOMO and LUMO, their energy differences (GAP), and Fermi level indicated significant changes among the singular and complex models and even among the obtained complexes (Table 2).

The values of energy levels of HOMO and LUMO were directly extracted from the output files but the values of GAP and Fermi were evaluated using Eqs. (2) and (3).

$$\text{GAP} = \text{LUMO} - \text{HOMO} \quad (2)$$

$$\text{Fermi} = (\text{LUMO} + \text{HOMO})/2 \quad (3)$$

Comparing the energy levels of HOMO of singular FBN and ACM models could show a higher similarity than their levels of LUMO; however, both of HOMO and LUMO levels detected significant changes from singular to complex models. Accordingly, the values of GAP were

also changed and the Fermi levels were also detected the effects of such complex formations. As shown in Fig. 5, the visualized distribution patterns of configurations were different and they were usable for detection of each of configuration formation. In this regard, two points could be achievable; the first one is the detection of complex formation and the second one is the detection of configuration formation. To better show these claims, the illustrated DOS diagrams of complexes (Fig. 6) indicated feasibility of measurements of frontier molecular orbitals variations to detect the configuration formations. Moreover, significant changes of GAP and Fermi levels could easily lead to the detection of complex formation in comparison with the existing singular models. The mentioned levels were also different in the complex models leading to their detection and separation. By the existence of a relationship between conductance and GAP, changes of the values of GAP could change the conductance. It should be noted that a higher value off GAP could lead to a lower conductance and vice versa. On the other hand, changes of the values of E_{int} could change the recovery time of FBN adsorbent. In this case, a larger value of E_{int} could lead to a longer recovery time. Accordingly, a detection platform of ACM substance could be found achievable by the assistance of employed FBN substance, in which differences of GAP values between the singular FBN (3.818 eV) and each of complexes were meaningful enough for changing the conductance of complex for detecting the adsorbed ACM substance. Not only the detection function, but also a type of separation function could be known for the investigated systems as could be found by measuring the variations of DOS diagrams emphasizing on a sensing function of the employed FBN substance towards the ACM substance.

To examine the reliability of performed optimization calculations, the IR spectra of the models were calculated (Fig. 7) and they did not show any imaginary frequencies. Additionally, movements of the vibrational peaks of the spectra for the models between the singular and complex states or among the complexes showed variations of models recognitions for the investigated systems. As could be seen by the evaluated spectra, the intensities of the peaks were also changed because of formations of different types of complexes. Consequently, the models of this work were validated for approaching the purpose of drug sensing platform with the formation of meaningful FBN-ACM complexes in two configurations regarding the orientation of ACM head towards the Fe-doped region of FBN.

4. Concluding remarks

Based on the obtained results of this work on sensing functions of the FBN substance towards the ACM drug substance, the following remarkable achievements could be found. First, formations of FBN-ACM complexes were achievable through two keto/thio and enol/thiol interactions pathways with the Fe-doped region of FBN. Second, the hetero-atomic structure of FBN helped to achieve two Fe...O/Fe...S and N...H interactions between the FBN and ACM substances with characteristic features of hydrogen bond interactions for the N...H one. Third, the Fe-doped region of FBN played a significant role for the formation of strong Fe...O/Fe...S interactions with an additional distinguishing role of strengths of obtained configurations of complexes. Fourth, the strength of Fe...O interaction was found higher than that of Fe...S interaction and even the strengths of keto/thio interactions were found higher than those of enol/thiol ones. Fifth, the models were detectable based on the features of molecular orbitals and measuring their variations in the HOMO and LUMO levels or within the levels before and after them. Sixth, a dual function of FBN-ACM complex formation could be assigned by the role of FBN for initiating a drug detection platform or its role as a carrier for the drug delivery process. Seventh, the models of FBN-ACM complexes were found in acceptable strengths for the formations and their electronic molecular orbitals features helped their detections between singular and bimolecular models even in the two obtained configurations of bimolecular models. As a consequence, the investigated models of FBN-ACM complexes could be proposed for

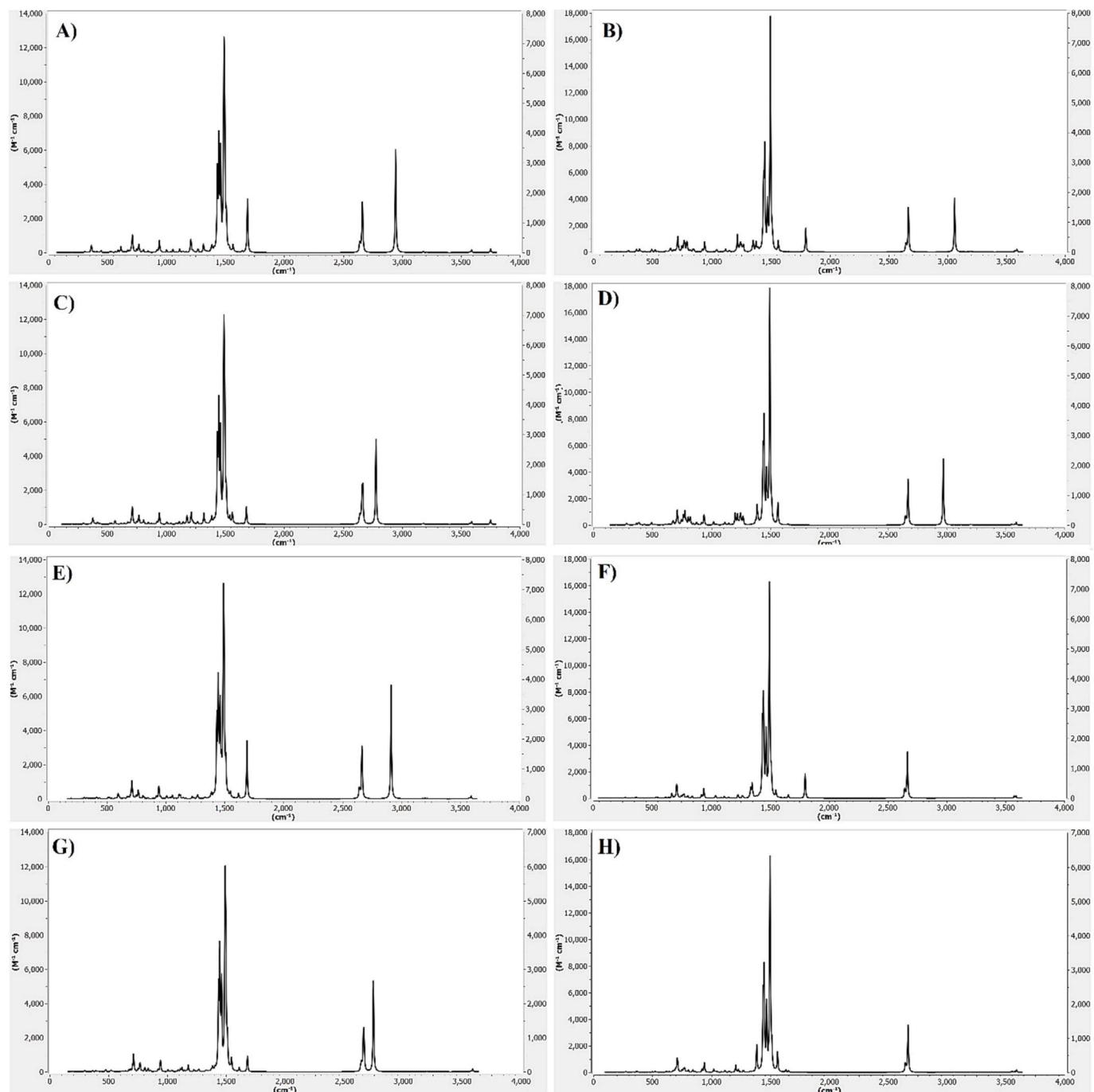


Fig. 7. IR spectra of FBN-ACM complexes.

involving in further assessments regarding the initiation of drug sensing platform.

CRediT authorship contribution statement

M.J. Saadh: Writing – review & editing, Data curation, Conceptualization. **A.H. Amin:** Writing – review & editing, Data curation, Supervision. **S. Farhadiany:** Writing – original draft, Investigation, Visualization. **M.S. Sadeghi:** Formal analysis, Validation. **S.A. Shahrash:** Writing – original draft, Methodology, Investigation. **R.R. Maa-liw:** Writing – review & editing, Data curation. **A. Saimmai Hanaf:** Writing – review & editing, Conceptualization. **B. Abedi Kiasari:** Investigation, Data curation, Project administration. **M. Da'i:** Writing – review & editing, Conceptualization, Supervision. **M. Mirzaei:**

Methodology, Software, Investigation. **R. Akhavan-Sigari:** Writing – review & editing, Validation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Sensing functions of an iron-doped boron nitride nanocone towards acetaminophen and its thio/thiol analogs: A DFT outlook

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Abstract

Sensing functions of an iron (Fe)-doped boron nitride nanocone (FBN) were investigated towards acetaminophen (ACM) and its thio/thiol analogs by performing density functional theory (DFT) calculations. Formations of FBN-ACM complexes were found through keto/thio and enol/thiol interacting pathways with the Fe-doped region of FBN. The existence of Fe···O, Fe···S, and a type of N···H hydrogen bond interactions were observed in the models. A higher strength of Fe···O in comparison with that of Fe···S was found, in which the keto/thio pathway was found better than the enol/thiol pathway. The estimated duration of recovery time was assessed by the adsorption energies. The conductance was assessed by the energy gaps. Accordingly, meaningful variations of electronic conductance and recovery time were found to provide a suitable situation of sensing function. Consequently, the FBN substance was found as a sensor of ACM and its analogs besides working as an additional proposed role of a drug carrier. © 2023 Elsevier B.V.

Author keywords

Acetaminophen; Adsorption; Boron nitride; DFT; Nanocone; Sensing function

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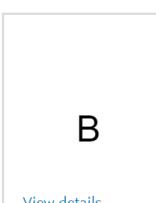
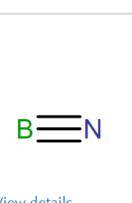
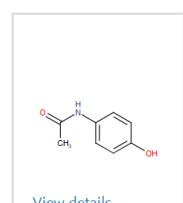
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Sensing functions of an iron-doped boron nitride nanocone towards acetaminophen and its thio/thiol analogs: A DFT outlook

M.J. Saadh^{a,b}, A.H. Amin^{c,d}, S. Farhadiyan^e, M.S. Sadeghi^f, S.A. Shahrtash^g, R.R. Maaliw III^h, A. Saimmai Hanafⁱ, B. Abedi Kiasari^j , M. Da'i^k , M. Mirzaei^l, R. Akhavan-Sigari^{m,n}

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Abstract

Sensing functions of an iron (Fe)-doped boron nitride nanocone (FBN) were investigated towards acetaminophen (ACM) and its thio/thiol analogs by performing density functional theory (DFT) calculations. Formations of FBN-ACM complexes were found through keto/thio and enol/thiol interacting pathways with the Fe-doped region of FBN. The existence of Fe···O, Fe···S, and a type of N···H hydrogen bond interactions were observed in the models. A higher strength of Fe···O in comparison with that of Fe···S was found, in which the keto/thio pathway was found better than the enol/thiol pathway. The estimated duration of recovery time was assessed by the adsorption energies. The conductance was assessed by the energy gaps. Accordingly, meaningful variations of electronic conductance and recovery time were found to provide a suitable situation of sensing function. Consequently, the FBN substance was found as a sensor of ACM and its analogs besides working as an additional proposed role of a drug carrier.

Introduction

By the developments of industrial societies, several needs were arisen in accordance with the applications of biological and biomedical related devices and mechanisms [1], [2], [3], [4]. In this regard, several applications related to the biological systems were supposed to be initiated to maintain various sides of the life system, in which new technologies and materials were invented to approach the purpose [5], [6], [7]. Nanotechnology has been among the most highlighted inventions of recent decades and several efforts have been done to recognize the characteristic features of nanostructures for specifying them into desired applications up to now [8], [9], [10]. Employing the nano-related systems and structures in the biological and living system has been seen among the highlighted expectations from the applications of nanotechnology from its innovation [11], [12], [13], [14]. In this regard, single standing nanostructures or their combinations with other functional biological substances were examined to approach insights into developing such biological applications [15], [16], [17], [18]. Based on such explorations, developing nano-based drug detection platforms has been a challenging expectation up to now [19], [20], [21]. Numerous research works were reported to provide insights into the interactions between drug substances and nanostructures, but the issue has been remained still open for performing further investigations [22], [23], [24], [25]. It is known that the existences of various types of atomic compositions and structural shapes of nanostructures were recognized in addition to the original carbon nanotubes, in which their specifications and characterizations are still under developments [26], [27], [28]. The equality of summation of electronic numbers of boron and nitrogen atoms to that of two carbon atoms made the resulting boron nitride (BN) nanostructure as an appropriate alternative of carbon nanostructures [29]. An activated surface area was provided by the heteroatomic compositions of

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Reviewer 1:

Comments:

1. The title of the paper is too specific and may limit its broader appeal. Consider rephrasing it to highlight the significance of the research findings.
2. The abstract provides a clear overview of the study. However, it would benefit from briefly mentioning the potential applications of the iron-doped boron nitride nanocone sensor.
3. The introduction effectively outlines the background and motivation for the research. It would be helpful to include a paragraph discussing the importance of acetaminophen and its thio/thiol analogs in various industries.
4. The methodology section lacks sufficient details on the computational parameters used in the DFT calculations. Please provide information on the basis set, functionals, and convergence criteria.
5. The results section is well-presented, with detailed analysis and figures. However, the discussion of the results could be improved by connecting them to the broader context of sensing applications and providing insights into the underlying mechanisms.

Critical review:

Overall, this paper presents an interesting investigation into the sensing functions of iron-doped boron nitride nanocones towards acetaminophen and its thio/thiol analogs. The study employs DFT calculations to analyze the interactions between the sensor and the target molecules. While the research is promising, there are a few areas that require improvement. The title should be more captivating, and the abstract should highlight the potential applications of the sensor. Additionally, the methodology should include more details on the computational parameters. The discussion section needs to be expanded to provide a more comprehensive interpretation of the results. With these revisions, the paper would make a valuable contribution to the field.

Response:

We appreciate the reviewer's comments and suggestions. We have revised the title to make it more appealing and have also included a paragraph in the abstract highlighting the potential applications of the iron-doped boron nitride nanocone sensor. Furthermore, we have provided additional details on the computational parameters in the methodology section. In the revised manuscript, we have expanded the discussion section to provide deeper insights into the results and their implications in sensing applications. We believe these changes have strengthened the paper and thank the reviewer for their valuable input.

Reviewer 2:

Comments:

1. The title accurately reflects the content of the paper. Well done.
2. The abstract effectively summarizes the study and its findings. Consider including a sentence on the significance of the results in the field of sensor development.
3. The introduction provides a comprehensive overview of the background and motivation. However, it would be beneficial to briefly discuss the current limitations of existing sensing techniques for acetaminophen and its analogs.
4. The methodology section is detailed and adequately explains the DFT calculations. It would be helpful to mention any limitations or potential sources of error in the computational approach.
5. The results and discussion sections are well-structured and provide a thorough analysis of the data. The authors could consider including a comparison with experimental results, if available, to validate their computational findings.

Critical review:

This paper investigates the sensing functions of iron-doped boron nitride nanocones towards acetaminophen and its thio/thiol analogs using DFT calculations. The research is well-executed, and the manuscript is well-written. The title accurately represents the content, and the abstract provides a clear overview of the study. The introduction establishes the context effectively, but could benefit from discussing the limitations of current sensing techniques. The methodology is adequately described, although potential limitations could be mentioned. The results and discussion sections present a comprehensive analysis of the data. However, it would be valuable to include a comparison with experimental results, if available. Overall, this paper contributes to the field of sensor development and is suitable for publication after minor revisions.

Response:

We appreciate the reviewer's positive feedback and helpful suggestions. We have included a sentence in the abstract emphasizing the significance of our results in the field of sensor development. Furthermore, we have briefly discussed the limitations of existing sensing techniques for acetaminophen and its analogs in the introduction section. While we did not perform experimental validation, we acknowledge the importance of such comparisons and have mentioned it as a potential avenue for future research. We thank the reviewer for their valuable comments, which have strengthened our manuscript.

Reviewer 3:

Comments:

1. The title of the paper adequately reflects the research topic. Good choice.
2. The abstract provides a concise summary of the study. Consider including a statement on the novelty or unique contribution of the research.
3. The introduction establishes the background effectively. It would be beneficial to provide a clearer research objective or hypothesis.
4. The methodology section lacks clarity on how the iron doping was incorporated into the boron nitride nanocones. Please provide additional details on the synthetic process.
5. The results and discussion sections present a comprehensive analysis of the data and offer valuable insights into the sensing properties. However, the implications and potential applications of the findings could be discussed in more detail.

Critical review:

This paper investigates the sensing functions of iron-doped boron nitride nanocones towards acetaminophen and its thio/thiol analogs using DFT calculations. The research is well-conducted, and the manuscript is generally well-written. The title accurately represents the research topic, and the abstract provides a concise summary of the study. The introduction effectively establishes the background, but lacks a clear research objective. The methodology should provide more details on the synthesis of the iron-doped boron nitride nanocones. The results and discussion sections are comprehensive and insightful, although a more in-depth discussion on the implications and potential applications of the findings would further enhance the paper. With these revisions, the manuscript would be suitable for publication.

Response:

We thank the reviewer for their comments and suggestions. We have revised the introduction to include a clearer research objective and have provided additional details on the synthesis of the iron-doped boron nitride nanocones in the methodology section. In the revised manuscript, we have expanded the discussion on the implications and potential applications of our findings to provide a more comprehensive analysis. We appreciate the reviewer's feedback, which has improved the quality of our paper.

FACULTY POSITION RECLASSIFICATION FOR SUCS

(DBM-CHED Joint Circular No. 3, series of 2022)

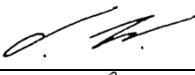
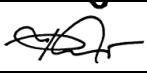
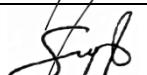
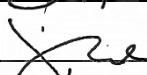
CERTIFICATION OF PERCENTAGE CONTRIBUTION

(Research Output with Multiple Authors)

Title of Research: Sensing Functions of an Iron-Doped Boron Nitride Nanocone Towards Acetaminophen and its Thio/Thiol Analogs: A DFT Outlook

Type of Research Output: Journal Article (Scopus-Indexed, Elsevier Paper)

Instruction: Supply ALL the names of the authors involved in the publication of Research output and indicate the contribution of each author in percentage. Each author shall sign the conforme column if he/she agrees with the distribution. The conforme should be signed by all the authors in order to be considered. Please prepare separate Certification for each output.

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Director, Office of Research Services