Boron nitride nanocone as an adsorbent and senor for Ampicillin: A Computational Study

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ABSTRACT

In this research, the performance of boron nitride nanocone for the detection and removal of ampicillin was investigated by infra-red (IR), natural bond orbital (NBO), frontier molecular orbital (FMO) computations. The calculated values of adsorption energy showed the interaction of ampicillin with BN nanocone is experimentally possible. The calculated values of Gibbs free energy and thermodynamic equilibrium constant showed the adsorption process is spontaneous and irreversible. The calculated values of enthalpy changes and specific heat capacity showed ampicillin adsorption is exothermic and BN nanocone can be used for the construction of a new thermal sensor for the detection of ampicillin. The effect of temperature on the thermodynamic parameters was also evaluated and the results indicated ampicillin adsorption is more favorable in room temperature. The NBO results demonstrated in both of the studied configurations a monovalent chemical bond is formed between the nanostructure and the adsorbate and the interaction process is chemisorption. The DOS spectrums showed the bandgap of BN nanocone increased from 1.888 (eV) to 7.030 (eV) which proved this nanomaterial is an appropriate electrochemical sensing material for detection of ampicillin. Some important structural parameters such as dipole moment, electrophilicity, maximum charge capacity, chemical hardness and chemical potential were also calculated and discussed in detail.

1. Introduction

Groundwater contamination by pharmaceutical ingredients is an environmental problem of widespread concern [1-2]. Residual pharmaceutical ingredients will be inevitably transported into biological wastewater treatment plants and have been recognized as part of the hazardous chemical substances able to alter the natural equilibrium system of the surrounding environment [3]. Recently, the presence of antibiotics in the environment has received much attention due to their impact on health and the environment because their presence in the waters provides the formation and development of antibiotic-resistant bacteria [4]. Therefore, it is of utmost importance to remove the antibiotic residues from the wastewater from sources such as households, hospitals and pharmaceutical factories before discharging them to the environment. Regular water and wastewater treatment may not be able to remove pharmaceutical compounds effectively. Accordingly, the development

of new and effective wastewater treatment technologies, such as biodegradation, hydrolysis, chemical oxidation, volatilization and adsorption have been intensively studied in the past decade [5-8]. Among these techniques, adsorption is preferred due to simplicity in design, ease of fabrication, high efficiency, relatively lower cost and absence of high toxic by-product [9]. Many polymeric and inorganic materials such as activated carbon [10], zeolite [11] and carbon nanotube [12], etc. have been proven to be effective for the absorption of the pollutants. However, they frequently suffer from the disadvantage of limited adsorption capacity or slow adsorption rate [13]. Therefore, novel adsorbent materials with high adsorption capacity and easy cycling ability still keep a challenge.Ampicillin (AM) (Figure 1) in its turn, is a β-lactam antibiotic of a large spectrum, able to interact with both gram-positive and gram-negative bacteria. Due to this characteristic, AM is largely applied to treat several kinds of conditions, like gonorrhea, urinary infections, ear, nose

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and throat infections [14-15]. It has been one of the most-consumed antibiotics worldwide, resulting in its detection in surface waters, sewage treatment plants and hospital effluents [16]. Some previous studies approached the removal of ampicillin and similar β-lactam antibiotics by adsorption. Weng et al. [17] studied simultaneous adsorption of amoxicillin, ampicillin and penicillin onto functional bentonite supported nanoscale Fe/Ni, reaching 80.6% removal in the mixture and 85.1% removal in the individual solution. Other researches evaluated the removal of ampicillin in different adsorbents, like ordered mesoporous silica and modified Ponorogo bentonite [14,18].

Boron nitride (BN), an environmentally benign material, has been demonstrated that porous BN nanomaterials can treat a wide range of pollutants (such as dyes, organic solvents, heavy metal ions, oils, etc.) from water [19]. They are similar to carbon nanomaterials in their geometrical structures and vary in their physicochemical properties. BN in nanoscale has different structures such as nanotubes, sheets, fullerenes, and nanocones. BN nanocones are another form of BN nanostructures. Boron-nitride nano-cones (BN nanocones) are discovered in 1994 as cap nanotubes end; then, they are synthesized as free structures by different groups. BN nanocones can be made by rolling nanostructure sheets. The characteristics of nanocones depend on the angle of the sector removed from a flat sheet to form a cone, namely, the disclination angle [20]. The BN nanocones have three types of covalent bonds; those are B-N, B-B, and N-N bonds which lead to differences in physical, chemical, and electronic properties between carbon and boron-nitride nanostructures [21-22]. The 240° disclination is the smallest cone geometry ensuring the presence of B-N bonds only (Figure 1). BN can be considered as promising adsorbent due to their high stability in harsh conditions, which enables more treatment techniques for recycled usage [23-24].

In this work, the electronic structure of a representative BN nanocone with 240° disclination was studied by density-functional theory (DFT) calculations and the performance of BN nanocones as an adsorbent and sensing material for detection and removal of Ampiciline was evaluated NBO, IR and FMO computations for the first time in this research.

2. Results and Discussion

2.1. NBO and Structural Analysis

As can be seen from Figure 2, in order to find the most stable configuration, the AM interaction with BN nanocone was evaluated at two different situations. In A-Conformer, the AM was inserted near the open end cap of BN nanocone while, in B-Conformer, the medicine molecule was placed near the outer surface of the nanocone towards its carbonyl group. Then, geometrical optimizations were performed on the designed structures. As the provided initial and optimized structures in Figure 2, show clearly after optimization BN nanocone experiences a tangible deformation in its structure which can be due to the formation of new bonds between the nanostructure and the adsorbate molecule. In addition, the calculated adsorption energy values in Table 1, (-337.067 and 137.574 kJ/mol for A and B conformers respectively) indicate the AM adsorption process is experimentally feasible and the adsorption process is likely to be chemisorption [25-30]. In this respect, to get better insights into the adsorption mechanism NBO computation were also done on the optimized structures and the results were presented in Table 1. As it is obvious, in both configurations a monovalent chemical bond with SP^3 hybridization and occupancy of 2 electrons are formed between the nano-adsorbent and ampicillin molecule [31]. Therefore, it seems BN nanocone is a suitable adsorbent for the removal of AM from environmental samples. The next matter that can be understood from the calculated values of total electronic energy and adsorption energy is that the AM interaction with the adsorbent is more favorable in A-Conformer because of more negative obtained values in this situation. The dipole moment was the next investigated parameter, as it is clear from Table 1, the dipole moment of AM increased sharply after its adsorption on the surface of BN nanocone which indicates AM –BN nanocone complexes are more soluble in water in comparison to the pure AM [32]. It should be noted that the calculated vibrational frequencies for all of the studied structures were in the range of 10.589 to 3126.543 cm^{-1} which indicates all of the evaluated structures are a true local minimum.
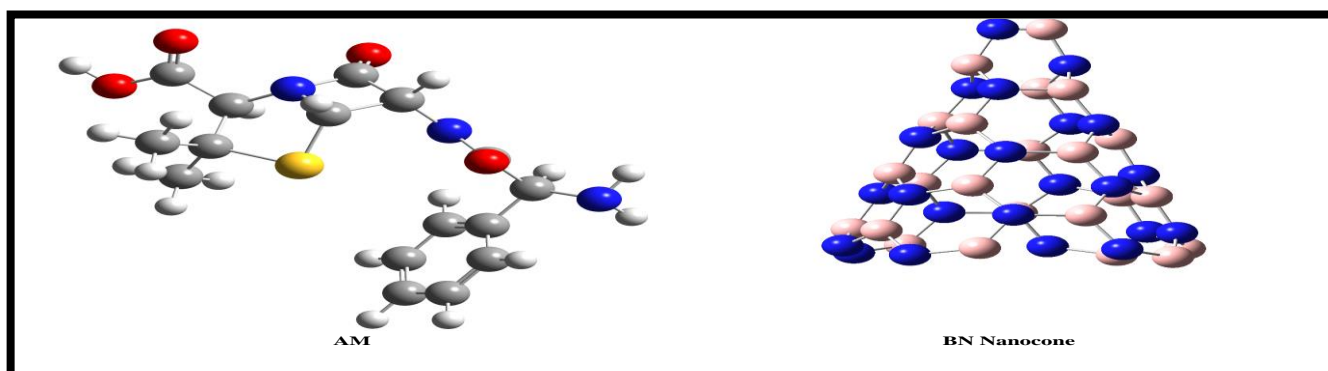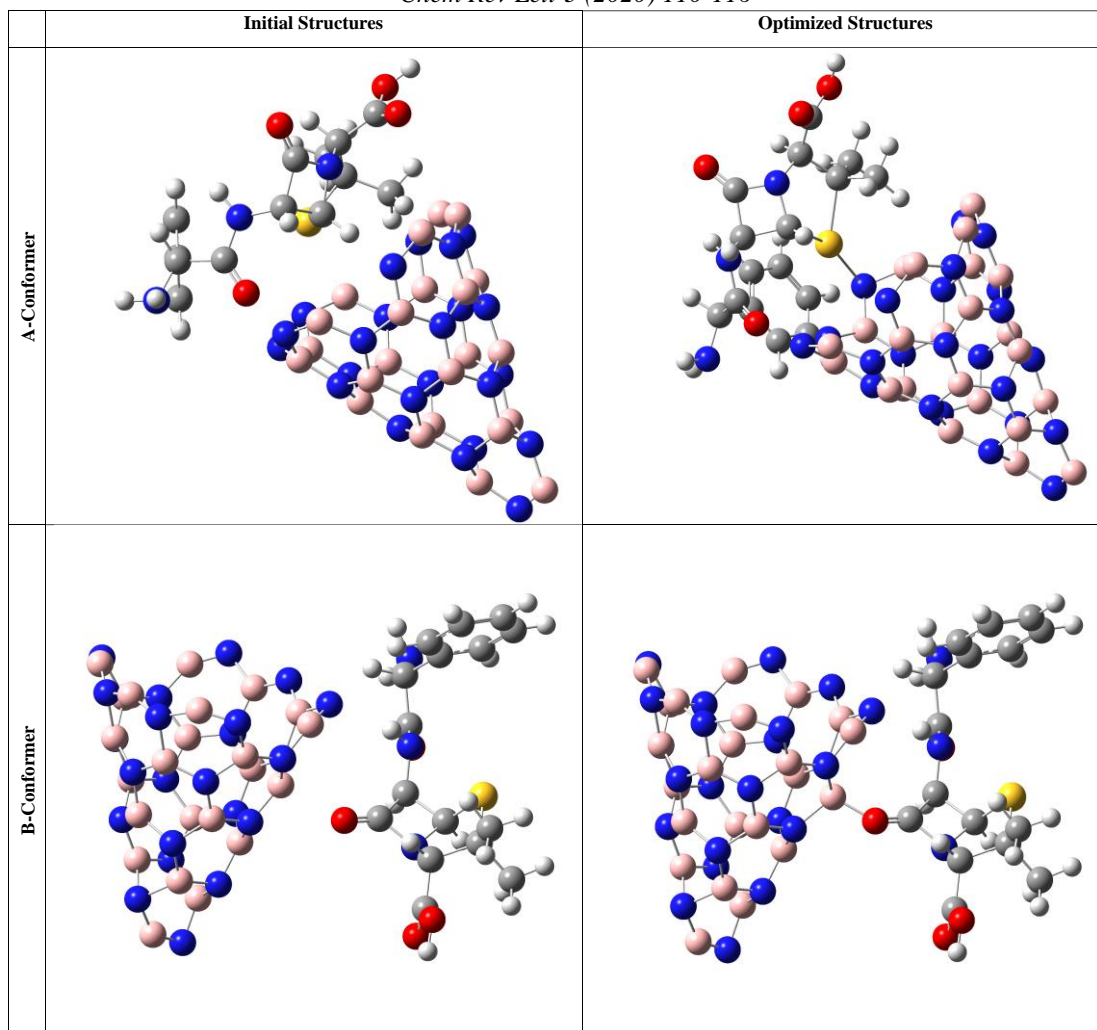

Figure 1. Optimized structure of AM and BN Nanocone

Figure 2. The Initial and optimized structures of AM-BN nanocone complexes

Table 1. The calculated values of bond lengths, bond order, occupancy, hybridization, bond energy, total electronic energy, adsorption energy, the lowest frequency, zero-point energy and dipole moment for AM, BN nanocone and their complexes

|		Bond length (Å)	Bond order	Occupancy	Hybridization	Bond energy (a.u.)	Total electronic energy (a.u)	Adsorption energy (kJ/mol)	The lowest frequency (cm⁻¹)	Zero-point energy (kJ/mol)	Dipole Moment (Deby)
AM	---	---	---	---	---	---	-1459.312	---	11.268	1045.58	3.430
BN Nanocone	---	---	---	---	---	---	-1798.737	---	75.428	724.21	6.340
A-Conformer	S-N	1.72	1	1.99	$Sp^{2.97}$	-0.464	-3258.178	-261.867	12.320	1777.62	27.120
B-Conformer	O-B	1.68	1	1.96	$Sp^{3.01}$	-0.512	-3258.102	-62.374	10.589	1775.97	17.890

2.2. Thermodynamic Studies

In order to evaluate the thermochemistry properties of the adsorption process and investigating the effect of temperature, the IR computations were performed on the structures and important thermodynamic parameters including the adsorption enthalpy changes (ΔH_{ad}), Gibbs free energy changes (ΔG_{ad}), the logarithm of thermodynamic equilibrium constants (K_{th}) and specific heat capacity (C_V) were calculated in the temperature

range of 298-398 K at 10° intervals and the results are presented in Figure 3. As can be seen, the values of ΔH_{ad} are negative for both of the configurations which indicate the AM interaction with BN nanocone is exothermic [33]. Besides, the specific heat capacity of the nanostructure increased sharply when the AM molecules adsorb on its surface which showed the thermal conductivity of BN nanocone improved significantly during its interaction process with AM

[34]. Therefore, it can be concluded that BN nanocone is an ideal sensing material for the construction of novel thermal sensors for the detection of AM [35]. İn this type of sensors, the desired analyte interacts with the recognition element of the sensor and their interaction should be highly exothermic or endothermic then, the

carried out changes in the temperature of the sensor microenvironment will be measured by a sensitive thermistor and it will be used as a signal for determining the concentration of analyte [36].
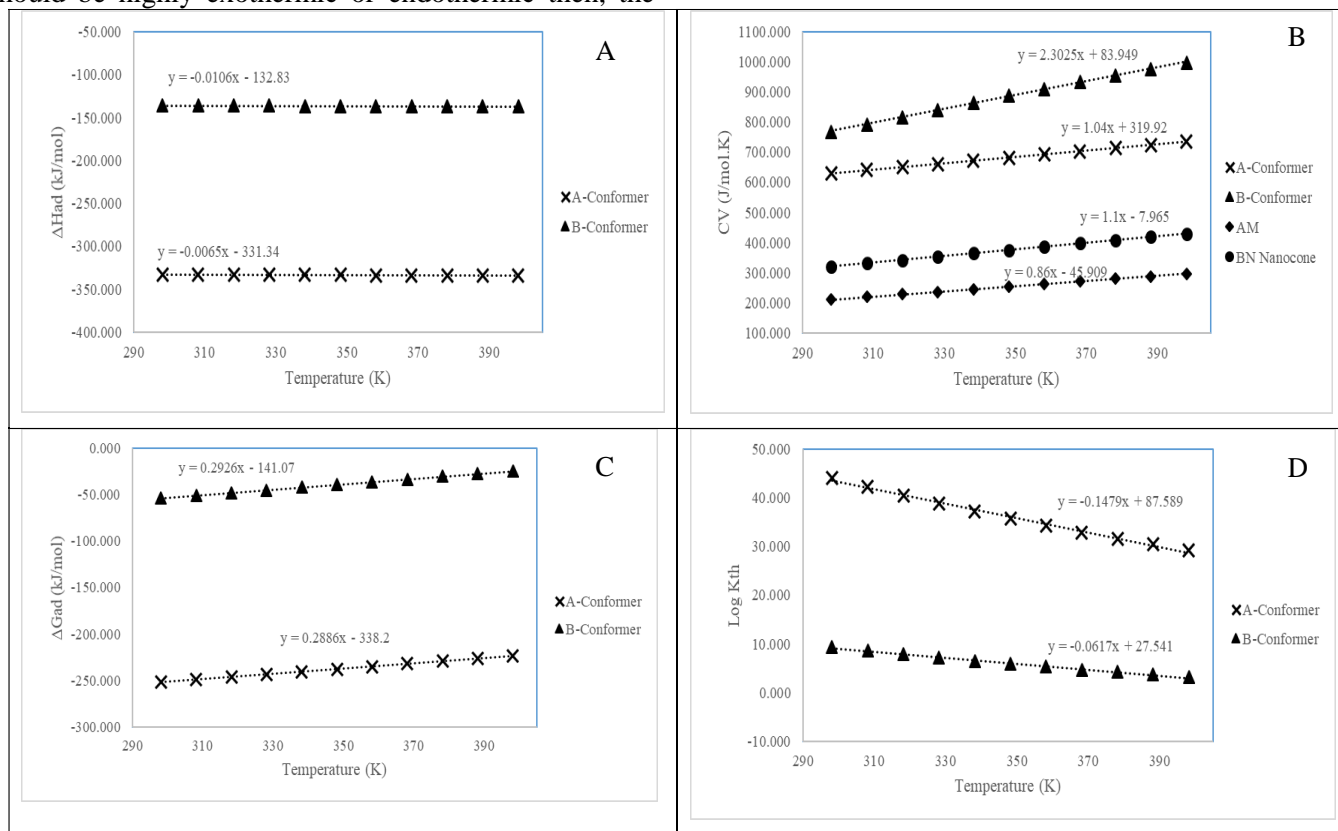
Figure 3. The calculated values of ΔH_{ad} (A), C_V (B), ΔG_{ad} (C) and the logarithm of K_{th} (D) as a function of temperature.

The calculated values of ΔG_{ad} and the logarithm of K_{th} showed the interaction of AM with BN nanocone is spontaneous and irreversible. The effect of temperature on these parameters was also checked out and the results showed by increasing of temperature, the ΔG_{ad} and Log K_{th} experienced a gradual increase and decrease respectively indicating the adsorption process is more favorable in lower temperatures [37, 38].

FMO Analysis

The energy discrepancy between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) is known as bandgap (E_g) in chemistry. This parameter has an inverse relationship with the electrical conductivity of compounds. İndeed, the molecules with lower values of bandgap will be more conductive than compounds with large bandgap [29, 30]. İn this respect, density of states (DOS) spectrums of AM, BN nanocone and their complexes were calculated and the results are presented in Figure 4. As it is clear, the bandgap of BN nanocone is 1.888 (eV) but when AM adsorbs on its surface, the

bandgap increases to 6.720 and 7.030 (eV) in A and B conformers respectively [31]. This phenomenon shows the electrical conductivity of BN nanocone decreased tangibly after the adsorption of AM and this reduction of conductivity can be used as a signal for the detection of AM in electrochemical sensors. Hence, BN nanocone is an appropriate sensing material for the development of new electrochemical sensors for the determination of AM [32].

The chemical hardness (η) and chemical potential (μ) of structures were also calculated and the results are given in Table 2. As can be seen, after the adsorption of AM on the surface of BN nanocone, the chemical hardness and chemical potential of AM experience a remarkable decline and increase respectively which indicates the reactivity of AM molecule enhances substantially when it adsorbs on the surface of the nanostructure because the molecules with low values of chemical hardness and high amounts of chemical potential are more reactive. After all, the essential electron transferrs for implementation of a chemical reaction can be done more easily in them [33].

The electrophilicity (ω) and maximum charge capacity (ΔN_{max}) were the last investigated parameters. Both parameters are good standards for estimating the tendency of a molecule towards an electron. İn fact, the compounds with higher values of ω and ΔN_{max} are more eager to absorb electron. As it is obvious from Table 2, the electrophilicity and maximum charge capacity of AM increase when it adsorbs on the surface of BN nanocone. Therefore, AM-BN nanocone complexes are more electrophile than pure AM [34].
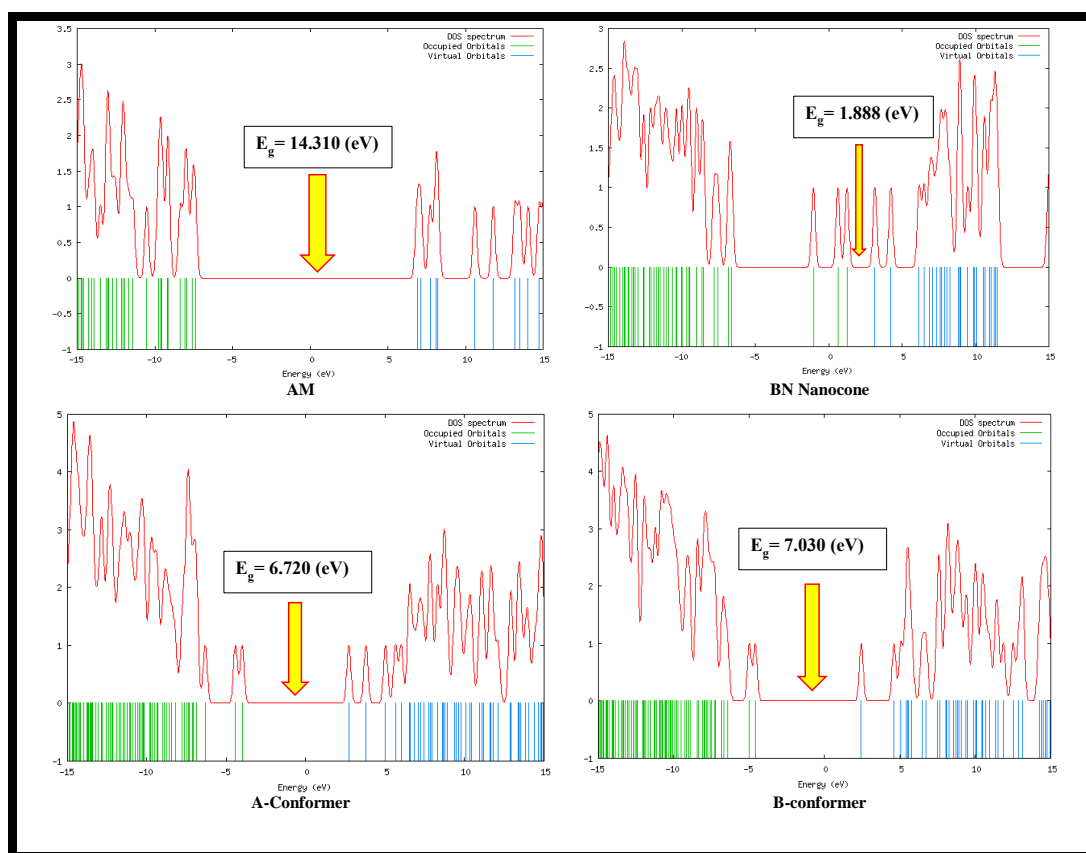
Figure 4. The DOS spectrums of AM, BN nanocone and their complexes

Table 2. The calculated values of HOMO and LUMO energy levels, bandgap, chemical hardness, chemical potenital, electrophilicity and maximum charge capacity for AM, BN nanocone and their complexes

	E_H (eV)	E_L (eV)	E_g (eV)	η (eV)	μ (eV)	ω (eV)	ΔN_{max} (eV)
AM	-7.410	6.900	14.310	7.155	-0.255	0.005	0.036
BN Nanocone	1.238	3.126	1.888	0.944	2.182	2.522	-2.311
A-Conformer	-4.010	2.710	6.720	3.360	-0.650	0.063	0.193
B-Conformer	-4.600	2.430	7.030	3.515	-1.085	0.167	0.309

3. Computational Details

The structures of BN nanocone, AM and their derived products were designed by Nanotube modeler 1.3.0.3 and GuassView 6 softwares [25, 26]. At first, all of the designed structures were optimized geometrically. Afterwards, IR, NBO and FMO computations were performed on them. All of the computations were done by Gaussian 16 software using the density functional theory method in the B3LYP/6-31G (d) level of theory [27]. This level of theory was selected because in former reports its results were in an admissible accordance with the experimental findings. GuassSum 3.0 software was employed for calculating the density of states (DOS) spectrums [28]. All of the calculations were implemented in the aqueous phase in the temperature range of 298-398 at 10˚ intervals.

The studied processes were as follows:

$$AM + BN\ Nanocone \rightarrow AM\text{-}BN\ Nanocone \quad (1)$$
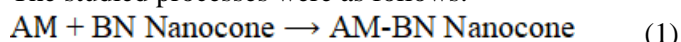
The values of adsorption energy values (E_{ad}) and thermodynamic parameters including adsorption enthalpy changes (ΔH_{ad}), Gibbs free energy changes (ΔG_{ad}) and thermodynamic equilibrium constants (K_{th}) were calculated by Equations 2-5 respectively.

$$E_{ad} = \left(E_{(\text{AM-BN Nanocone})} - \left(E_{(\text{AM})} + E_{(\text{BN Nanocone})} + E_{(\text{BSSE})} \right) \right) \quad (2)$$

$$\Delta H_{ad} = \left(H_{(\text{AM-BN Nanocone})} - \left(H_{(\text{AM})} + H_{(\text{BN Nanocone})} \right) \right) \quad (3)$$

$$\Delta G_{ad} = \left(G_{(\text{AM-BN Nanocone})} - \left(G_{(\text{AM})} + G_{(\text{BN Nanocone})} \right) \right) \quad (4)$$

$$K_{th} = \exp\left(-\frac{\Delta G_{ad}}{RT} \right) \quad (5)$$

In the referred equations, E is the total electronic energy of each structure, E_{BSSE} denotes the basis set superposition correction, H stands for the sum of the thermal correction of enthalpy and total energy of the evaluated materials. The G denotes the sum of the thermal correction of Gibbs free energy and total energy for each of the studied structures. R is the ideal gas constants, T denotes the temperature and S is the thermal correction of entropy for each structure [29-31]. Frontier molecular orbital parameters including bandgap (E_g), chemical hardness (η), chemical potential (μ), electrophilicity (ω) and the maximum charge capacity (ΔN_{max}) were calculated by equations 6-10 [32].

$$Eg = E_{LUMO} - E_{HOMO} \quad (6)$$

$$\eta = \left(E_{LUMO} - E_{HOMO} \right) / 2 \quad (7)$$

$$\mu = \left(E_{LUMO} + E_{HOMO} \right) / 2 \quad (8)$$

$$\omega = \mu^2 / 2\eta \quad (9)$$

$$\Delta N_{max} = -\mu / \eta \quad (10)$$

E_{LUMO} and E_{HOMO} in equations 6 to 10 are the energy of the lowest unoccupied molecular orbital and the energy of the highest occupied molecular orbital respectively [33, 34].

4. Conclusion

Removal of ampicillin is of great importance. İn this respect, the performance of BN nanocone as an adsorbent and sensor for this antibiotic was investigated theoretically by IR, NBO and FMO computations. The calculated thermodynamic parameters and adsorption energy values proved AM interaction with BN nanocone is exothermic, spontaneous, irreversible and experimentally possible and BN nanocone is an appropriate adsorbent for removal of AM. The values of specific heat capacity and DOS spectrums showed this nanomaterial is an appropriate thermal and electrochemical sensing material for the construction of novel sensors for the detection of AM. The NBO results indicated a monovalent chemical bond is created between AM and BN nanocone and their interaction is chemisorption.

Acknowledgements

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