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RESEARCH ARTICLE

Norfloxacin Adsorption on the Surface of $B_{12}N_{12}$ and $Al_{12}N_{12}$ Nanoclusters: A Comparative DFT Study

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ABSTRACT

A recent study conducted using density functional theory computations has shed light on the potential use of $B_{12}N_{12}$ and $Al_{12}N_{12}$ nanoclusters as adsorbents and sensing materials for the removal and electrochemical detection of norfloxacin (NFX). The results of the study indicated that both $B_{12}N_{12}$ and $Al_{12}N_{12}$ nanoclusters are feasible options for the removal of NFX, with $B_{12}N_{12}$ being more suitable as an adsorbent and $Al_{12}N_{12}$ being a better option as a sensing material for electrochemical detection. The thermodynamic parameters of the study showed that NFX adsorption on $B_{12}N_{12}$ is a spontaneous, exothermic, and one-sided process, while its interaction with $Al_{12}N_{12}$ is thermodynamically possible, two-sided, and equilibrium. The calculated frontier molecular orbital (FMO) analysis also revealed that both nanoclusters experienced a decrease in bandgap, with $Al_{12}N_{12}$ experiencing a sharper decline, indicating its suitability as a sensing material. Furthermore, the study found that NFX adsorption on the surface of both nanoadsorbents is more favorable at lower temperatures. This finding provides valuable insights into the potential use of these nanoclusters in NFX removal and electrochemical detection.

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INTRODUCTION

Antibiotics have long been a crucial component in modern medicine, saving countless lives by fighting off bacterial infections [1-3]. However, their widespread use has led to a concerning environmental issue - antibiotic contamination [4-6]. This contamination poses a significant threat to both human health and the health of other living organisms, as it can lead to antibiotic resistance and adverse side effects [7-10]. One such antibiotic that has been identified as a major environmental contaminant is norfloxacin (NFX, Fig. 1.) [11]. This fluoroquinolone antibiotic is highly effective against both gram-positive and gram-negative microbe infections, but its adverse effects include depression, nausea, vertigo, headache, hallucinations, tremor, and insomnia [12-16]. As such, it is crucial to set up a stragtforward, fast, and reproducible technique for its removal and determination.

Several methodolgies have been developed for the measurement of NFX, such as UV-Visible spectrophotometry [17], High-performance liquid chromatography [18], liquid chromatography-tandem mass spectrometry (LC-MS) [19], capillary electrophoresis [20], and fluorimetry [21]. However, these techniques suffer from various disadvantages such as being time-consuming, demanding high-cost and intricate instrumens, consuming large volumes of hazardous organic

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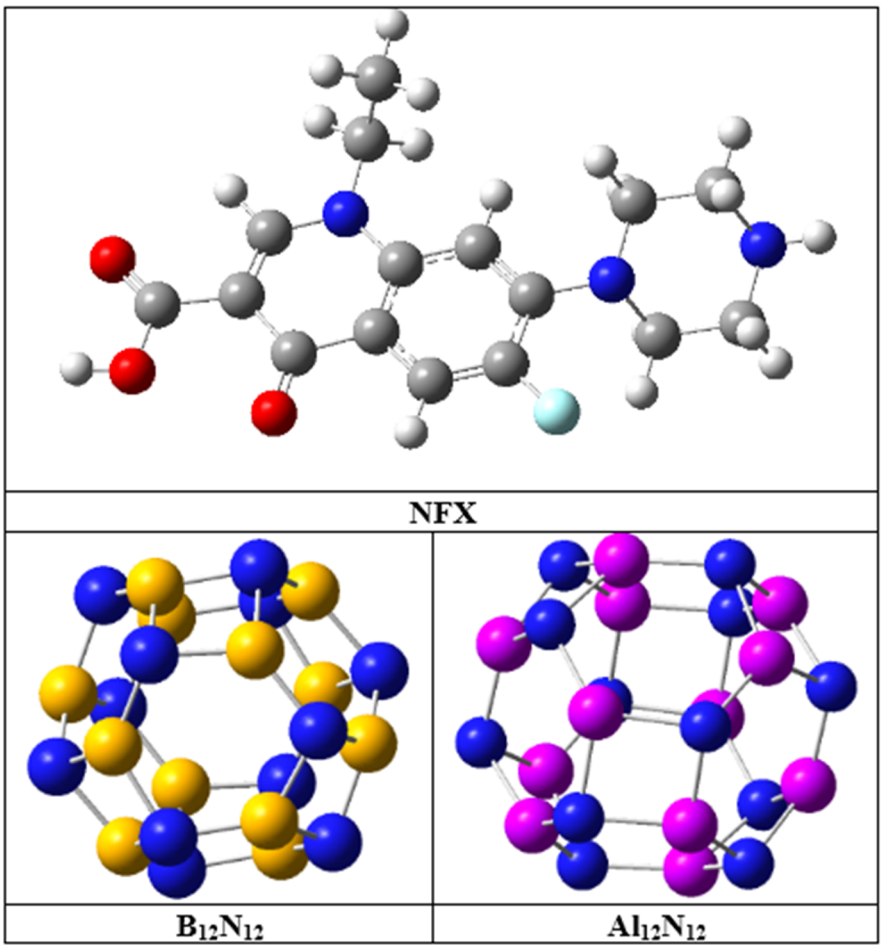

Fig. 1. The optimized structures of $B_{12}N_{12}$, $Al_{12}N_{12}$, and NFX (oxygen: red, nitrogen: blue, carbon: gray, hydrogen: white, fluorine; green, boron: yellow, aluminum: purple)

solvent, and demandig experienced staff for doing sample preparation and analysis steps [22, 23]. An alternative to these techniques is the use of electrochemical sensors. These sensors offer several advantages over traditional analytical techniques, including portability, simple and economic instrumentation, high selectivity and sensitivity, time-saving analysis procedure, and applicability in opaque and colored samples [24]. Electrochemical sensors can be used to detect NFX in environmental matrices with addmisible accuracy and precision, making them a prominent alternative for the determination of this antibiotic [25].

Different techniques have been established for the removal of NFX from effluents, including biological treatment [26], membrane filtration [27], and electrochemical destruction [28]. However, these techniques suffer from various disadvantages such as high cost, limited removal capacity, harsh reaction mediums, and being time-consuming [28]. Therefore, alternative techniques are being explored to overcome these limitations. On the other hand, sdsorption is a highly efficient and cost-effective technique that has gained popularity in recent times due to its versatility and ease of operation [29]. One of the major advantages of adsorption is its ability to remove hazardous materials from various sources such as air, water, and soil [29]. Adsorption also offers flexibility in terms of the chemical and physical features of the adsorbent used [29]. Another advantage of adsorption is its rapidness [29]. The process can be completed within a short period, making it ideal for applications that require quick results. Additionally, adsorption is easy to operate, making it accessible to a wide range of users [29]. Adsorption is a process in which molecules

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or particles are removed from a liquid or gas phase by adhering to the surface of a solid material called an adsorbent [30]. The adsorbent can be natural or synthetic and can be designed to target specific pollutants [31]. Adsorption has been shown to be effective in the removal of NFX from wastewater. The adsorbent material used for this purpose should have high reusability, admissible selectivity and repeatability [32]. The election of the adsorbent material is contingent on various parameters like cost, availability, and effectiveness [32].

In the realm of electrochemical sensor development, the first and most crucial step is identifying a material that exhibits a strong and selective interaction with the desired compound [33]. Recent molecular simulations have highlighted the potential of X_nY_n semiconductors (where X = B, Al, and Y = N, P) in this regard, specifically pointing towards the fullerene-like $X_{12}Y_{12}$ cages as particularly stable and promising candidates [34]. Of these fullerene-like nano-cages, $Al_{12}N_{12}$ and $B_{12}N_{12}$ (Fig. 1) stand out due to their exceptional stability, large band gap, and excellent surface area [35]. These unique characteristics make them ideal for a wide range of applications, including molecule electronic devices, biomedical engineering, sensing, and nanotechnology [36]. Given their potential, this study was sought to investigate the performance of $Al_{12}N_{12}$ and $B_{12}N_{12}$ fullerene-like nanocages as both an adsorbent and sensing material for the detection and removal of NFX using density functional theory computations.

COMPUTATIONAL METHODS

In this study, we utilized the software versions GuassView 6 [37] and Nanotube modeler 1.3.0.3 [38] to design the structures of $B_{12}N_{12}$, $Al_{12}N_{12}$, and NFX, along with their complexes. To ensure the accuracy of our results, each of the structures was first subjected to geometric optimization. We then performed computations for infra-red (IR), frontier molecular orbital (FMO), and natural bond orbital (NBO) on the designed structures. The density functional theory (DFT) method was used throughout the computations by Gaussian 16 software [39] at the B3LYP/6-31G (d) level of theory [40]. This level was selected due to its acceptability and consistency with experimental results from earlier studies. All computations were performed in a vacuum between 298 and 398 K at intervals of 10˚. The following processes were investigated [40]:

$$\text{NFX} + \text{Adsorbent} \rightarrow \text{NFX-Adsorbent} \quad (1)$$

The computed parameters including Adsorption energy values (E_{ad}), dipole moment, thermodynamic equilibrium constant (K_{th}), Gibbs free energy changes (G_{ad}), and adsorption enthalpy changes (H_{ad}), bandgap (E_g), chemical hardness (η), chemical potential (μ), maximum charge capacity (ΔN_{max}), and the electrophilicity (ω) were calculated as explained in [41-44].

RESULTS AND DISCUSSION

Structural and NBO Analysis

The optimized structures of the complexes were analyzed to determine the most stable configuration (Fig. 2.) [45]. It was found that NFX-$B_{12}N_{12}$ complexes experienced sharp structural distortions, while NFX-$Al_{12}N_{12}$ complexes did not undergo any structural deformations after geometric optimization. The calculated total electronic and adsorption energies (Table. 1) showed that NFX interaction with both adsorbents is experimentally possible, with NFX-$B_{12}N_{12}$ interaction being stronger than its interaction with $Al_{12}N_{12}$ [46]. The optimized structures were also subjected to IR computations and no negative vibrational frequency was observed, indicating that all the investigated structures are true local minimums [47]. The dipole moment of the scrutinized structures was also calculated, and the achieved results showed that NFX complexes with $B_{12}N_{12}$ and $Al_{12}N_{12}$ have higher dipole moment values than the pure drug molecule without the nanostructure, indicating the chemical reactivity and solubility of NFX improve after interacting with both nanocages [48]. Natural bond orbital (NBO) computations were also performed on the optimized structures to obtain more insights into the adsorption mechanism (Table. 2). The obtained results showed that in NFX-$B_{12}N_{12}$ complexes, a monovalent chemical bond with SP^3 hybridization has been formed between NFX and $B_{12}N_{12}$, indicating that NFX interaction with boron nitride nanocage is chemisorption [49]. However, no bond has been formed between NFX and $Al_{12}N_{12}$, implying that their interaction is physisorption. Overall, the study provides valuable insights into the interaction between NFX and different nanostructures, which can also help in developing more efficient drug delivery systems.

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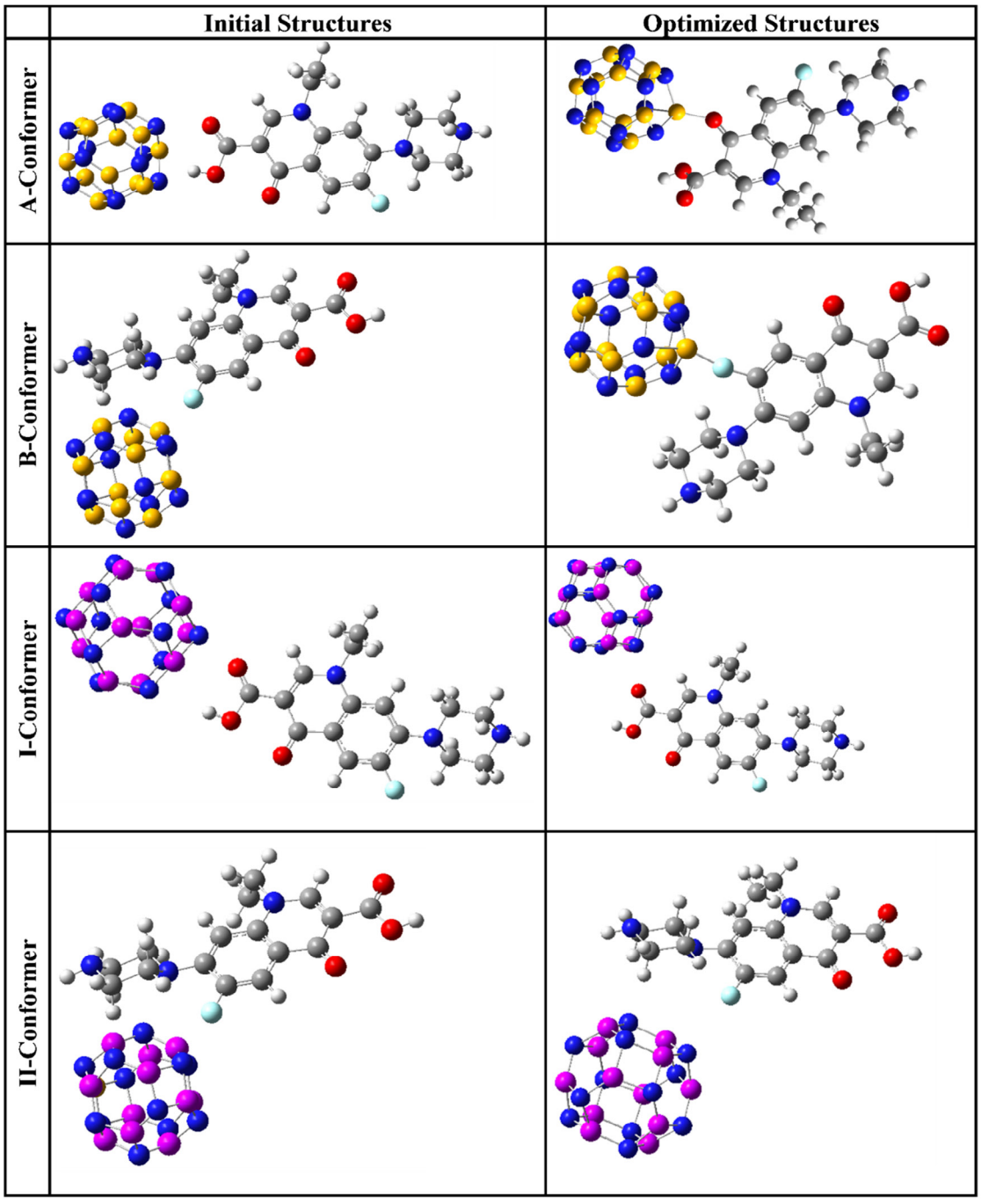

Fig. 2. Initial and optimized structures of NFX complexes with $B_{12}N_{12}$, and $Al_{12}N_{12}$ (oxygen: red, nitrogen: blue, carbon: gray, hydrogen: white, fluorine; green, boron: yellow, aluminum: purple

Thermodynamic Parameters

Adsorption is a process that involves the adhesion of molecules or particles to a surface. It is widely used in various applications such as wastewater treatment, gas separation, and drug delivery [43]. In recent years, nanocages have been developed as promising adsorbents due to their unique properties such as high surface area, tunable pore size, and excellent stability [44]. In this study, we investigated the thermodynamic parameters of the NFX adsorption process on both $B_{12}N_{12}$ and $Al_{12}N_{12}$ nanocages. The thermodynamic

Table 1. The values of total electronic energy, adsorption energy, zero-point energy (ZPE), the maximum and minimum IR frequencies and dipole moment for NFX, $B_{12}N_{12}$, $Al_{12}N_{12}$ and their complexes

NO	Total electronic energy (a.u)	Adsorption energy (kJ/mol)	ZPE (kJ/mol)	ν_{min} (cm^{-1})	ν_{max} (cm^{-1})	Dipole Moment (Debye)
NFX	-1089.778	---	1013.590	27.786	4241.629	5.140
$B_{12}N_{12}$	-938.547	---	391.630	369.919	1653.384	0.000
A-Conformer	-2028.418	-252.683	1411.310	16.376	4259.336	7.760
B-Conformer	-2028.389	-176.544	1409.680	9.536	4245.988	9.150
$Al_{12}N_{12}$	-3514.214	---	260.380	192.232	1204.272	0.000
I-Conformer	-4604.024	-92.281	1277.320	10.314	4243.369	16.230
II-Conformer	-4604.039	-130.884	1278.970	9.801	4240.210	12.840

Table 2. The NBO results for NFX-$B_{12}N_{12}$ complexes

NO		Bond length (A)	Bond order	Occupancy	Hybridization	Bond energy (a.u)
A-Conformer	B-F	1.823	1.000	1.994	$SP^{2.99}$	-0.237
B-Conformer	B-O	1.765	1.000	1.998	$SP^{2.98}$	-0.182

parameters including ΔH_{ad}, ΔG_{ad}, ΔS_{ad}, and Log K_{th} were calculated in the temperature range of 298-398 K at 10° intervals (Fig. 3.). The obtained results showed that the NFX interaction with both $B_{12}N_{12}$ and $Al_{12}N_{12}$ nanocages is exothermic and spontaneous at all studied conformers [45]. This indicates that the adsorption process is energetically favorable. The positive values of ΔS_{ad} showed that the adsorption procedure is favorable in terms of entropy, indicating that the disorderliness has increased [46]. This suggests that the NFX molecules are more disordered when adsorbed on the nanocage surface than in the bulk phase [46]. The high values of Log Kth for NFX-$B_{12}N_{12}$ complexes demonstrate that the NFX interaction with $B_{12}N_{12}$ is irreversible and non-equilibrium. On the other hand, the low amounts of Log Kth for NFX-$Al_{12}N_{12}$ complexes show that the NFX interaction with $Al_{12}N_{12}$ is reversible and equilibrium. The effect of temperature on all studied thermodynamic parameters was also investigated. The results showed that the adsorption process is more favorable at lower temperatures for both of the studied adsorbents [47]. This is because by increasing the temperature, ΔH_{ad} and ΔG_{ad} experienced a tangible incrementing, while ΔS_{ad} and Log K_{th} parameters decreased remarkably [47].

FMO Analysis

Electrochemical sensing materials have become increasingly important in the detection of various substances, including drugs and toxins. One key factor in determining the effectiveness of these materials is their electrical conductivity, which is inversely related to their band gap [48]. Materials with a narrow band gap tend to have higher electrical conductivity than those with a wide one [49]. To assess the efficiency of $B_{12}N_{12}$ and $Al_{12}N_{12}$ as electrochemical sensing materials for the detection of NFX, their band gap was computed. The results (Table. 3.) showed that the band gap of boron nitride nanocage was 6.830 (eV), while that of aluminum nitride nanocage was 3.930 (eV), indicating that the latter is more conductive than the former [43]. When NFX is adsorbed on the surface of $B_{12}N_{12}$, the band gap declines slightly, indicating that the electrical conductivity of $B_{12}N_{12}$ does not change significantly during the adsorption process, making it unsuitable for the detection of NFX [44]. On the other hand, the band gap of $Al_{12}N_{12}$ experienced a significant decrease when NFX adsorbs on its surface, indicating that its electrical conductivity enhances substantially, making it an excellent electrocatalytic modifier for the electrochemical detection of NFX [45].

In addition to band gap, other chemical properties such as electrophilicity, chemical hardness, maximum transferred charge capacity, and chemical potential were also calculated to determine the molecular properties. The results showed that after interacting with both nanocages, NFX's chemical hardness declines significantly, making it softer and more reactive than pristine NFX that does not contain a nano adsorbent

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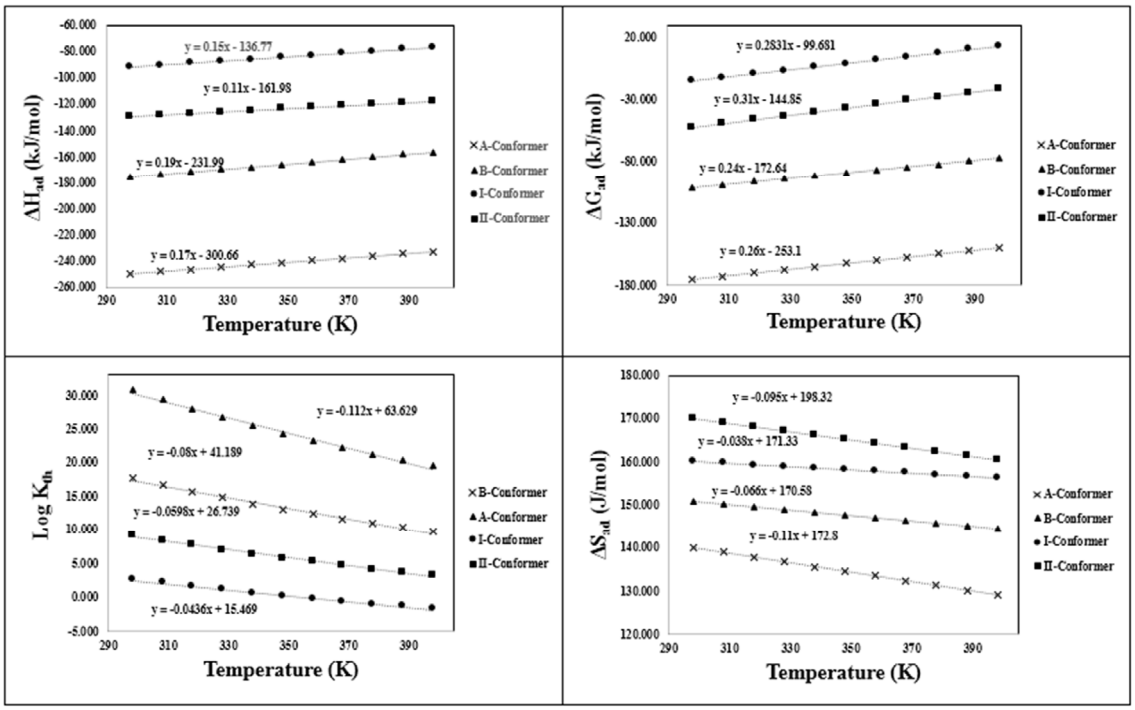

Fig. 3. Thermodynamic parameters of NFX adsorption process on $B_{12}N_{12}$, and $Al_{12}N_{12}$ including ΔH_{ad}, ΔG_{ad}, ΔS_{ad}, and the logarithm of K_{th} in the temperature 298-398 K at 10° intervals

Table 3. The calculated FMO parameters for NFX, NFX, $B_{12}N_{12}$, $Al_{12}N_{12}$ and their complexes

NO	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)	$\%\Delta E_g$	η (eV)	μ (eV)	ω (eV)	ΔN_{max} (eV)
NFX	-5.740	5.730	11.470	---	5.735	-0.005	0.000	0.001
$B_{12}N_{12}$	-7.700	-0.870	6.830	---	3.415	-4.285	2.688	1.255
A-Conformer	-4.327	2.233	6.560	-3.953	3.280	-1.047	0.167	0.319
B-Conformer	-3.656	2.817	6.472	-5.238	3.236	-0.419	0.027	0.130
$Al_{12}N_{12}$	-6.470	-2.540	3.930	---	1.965	-4.505	5.164	2.293
I-Conformer	-1.293	1.070	2.363	-39.864	1.182	-0.112	0.005	0.094
II-Conformer	-1.130	1.007	2.137	-45.632	1.068	-0.062	0.002	0.058

[46]. All investigated structures have a negative measured chemical potential, suggesting that they all have thermodynamic stability [47]. Furthermore, after interacting with both nanocages, both electrophilicity and maximum transferred charge capacity indices increased, indicating that NFX complexes with both nanocages have higher electrophilicity and are more likely to absorb electrons compared to pristine NFX [48].

CONCLUSION

A study was conducted to investigate the potential use of nanoclusters, specifically $B_{12}N_{12}$ and $Al_{12}N_{12}$, as an adsorbent and sensing material for the removal and detection of the highly consumed antibiotic NFX. The adverse effects of NFX on both the environment and human health have raised concerns, making its detection and removal crucial. The study found that NFX interaction with $B_{12}N_{12}$ is possible, but the existing interactions between the adsorbent and adsorbate were too strong and had a non-equilibrium nature. Thus, $B_{12}N_{12}$ was deemed appropriate for the removal of NFX, but not for its electrochemical detection. On the other hand, NFX showed a reversible and feasible adsorption behavior towards $Al_{12}N_{12}$. The bandgap of $Al_{12}N_{12}$ experienced a significant decline during the adsorption procedure of NFX, making it an

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ideal electrocatalytic sensing material for the development of novel electrochemical sensors for the detection of NFX. These findings highlight the potential use of $B_{12}N_{12}$ as an appropriate adsorbent for the removal of NFX and $Al_{12}N_{12}$ as an ideal electrocatalytic sensing material for the development of novel electrochemical sensors for the detection of NFX. However, further evaluation by experimental chemists is recommended to confirm these findings.

CONFLICTS OF INTEREST

The authors declare that they have no conflicts of interest.

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