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RESEARCH ARTICLE

Chloralhydrate Adsorption on the Surface of $C_8B_6N_6$ Nanocluster: A DFT Outlook

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ABSTRACT

In this study, the adsorption behavior of chloral hydrate (CH), a toxic sedative and potential environmental contaminant, on a $C_8B_6N_6$ fullerene-like nanocluster was systematically investigated using Density Functional Theory (DFT). Geometry optimizations and frequency calculations were performed at the B3LYP/6-31G* level to explore structural, electronic, and thermodynamic properties in both gaseous and aqueous phases. Three adsorption configurations were analyzed to determine the most stable conformer. The calculated adsorption energies were negative for all configurations, confirming the feasibility of the adsorption process. Among them, the B-conformer exhibited the strongest interaction, with adsorption energies of −102.395 kJ/mol in vacuum and −52.510 kJ/mol in water. The relatively moderate adsorption energies (<150 kJ/mol), absence of bond formation in NBO analysis, and minimal structural distortion indicate that the interaction mechanism is predominantly physisorption. Thermodynamic analyses revealed negative ΔH_ad and ΔG_ad values across the temperature range of 298–318 K, confirming that the adsorption process is exothermic and spontaneous, while lower temperatures favor stronger interactions. Frontier molecular orbital (FMO) analysis demonstrated a significant reduction in the band gap of $C_8B_6N_6$ upon CH adsorption (up to ~52% for the B-conformer), indicating enhanced electronic sensitivity and charge transfer capability. Additionally, adsorption reduced chemical hardness and increased electrophilicity, suggesting improved reactivity and sensing potential. These findings highlight the promising capability of $C_8B_6N_6$ nanoclusters for chloral hydrate adsorption and detection, offering valuable insights for the design of boron nitride-based nanomaterials in environmental remediation and sensor applications.

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INTRODUCTION

Chloral hydrate (CH) is a sedative and hypnotic compound that has been used in medicine for over a century, primarily for its calming and sleep-inducing effects [1]. Chemically, it is a chlorinated derivative of acetaldehyde, and it appears as a colorless crystalline solid that is soluble in water and alcohol [2]. Despite its historical use in treating insomnia and as an anesthetic adjunct, its toxicity and potential for misuse have raised significant concerns [3]. CH can be toxic when consumed in

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excessive amounts, leading to symptoms such as respiratory depression, gastrointestinal distress, cardiac arrhythmias, and even fatal overdose in severe cases [4]. It is metabolized in the body to trichloroethanol, which contributes to its sedative effects but also plays a role in its toxicity [5]. CH can occur as a contaminant or by-product in industrial processes involving chlorinated solvents, making it a potential environmental pollutant [6]. Its presence in water sources or industrial effluents highlights the importance of monitoring and determining its concentration to ensure public safety and environmental protection [7]. Therefore, determination and removal of CH is of great significance. Pharmaceuticals removal from water and wastewater has become a critical environmental concern due to the increasing presence of these contaminants, which can harm aquatic ecosystems and potentially affect human health [8]. Various techniques, such as advanced oxidation processes (AOPs) [9], membrane filtration [10], and biological treatments [11], have been employed to address this issue. However, many of these methods come with significant disadvantages [12]. AOPs, for instance, often require high energy input and the use of expensive chemicals, making them costly and less sustainable in the long term [13]. Membrane filtration, while effective in removing a wide range of contaminants, faces challenges such as membrane fouling, high operating costs, and the generation of concentrated waste streams that require further treatment [14]. Biological treatments, though environmentally friendly, are often limited by the inability of microorganisms to degrade certain pharmaceutical compounds completely, leading to partial treatment and potential formation of harmful by-products [15]. In contrast, adsorption has emerged as a promising alternative for pharmaceutical removal due to its numerous advantages [18]. This technique is highly efficient in capturing a wide range of pharmaceutical compounds, even at low concentrations, through the use of adsorbents such as activated carbon, biochar, or novel nanomaterials [19]. Adsorption processes are relatively simple to operate and do not require complex infrastructure or high energy input, making them cost-effective and sustainable [20]. Additionally, adsorption does not produce harmful by-products or secondary pollution, unlike some chemical methods [21]. The reusability and regeneration of certain adsorbents further enhance the economic and environmental viability of this approach [22]. Overall, adsorption stands out as a practical and efficient solution for addressing pharmaceutical contamination in water systems, overcoming many of the limitations associated with other removal techniques [23]. Pharmaceutical determination techniques play a crucial role in ensuring the safety, efficacy, and quality of drugs [24]. Traditional methods such as spectrophotometry, chromatography, and mass spectrometry have been widely used due to their high sensitivity and ability to provide detailed chemical information [25]. However, these techniques often come with significant disadvantages, including high operational costs, lengthy preparation times, complex sample processing, and the need for highly trained personnel to operate the sophisticated instrumentation [26]. Additionally, many of these methods require the use of hazardous chemicals and solvents, raising environmental and safety concerns [27]. On the other hand, electrochemical sensors have emerged as a promising alternative with several distinct advantages [28]. These sensors are cost-effective, portable, and easy to use, making them particularly suitable for on-site and real-time pharmaceutical analysis [29]. They offer rapid response times and high selectivity while requiring minimal sample preparation [30]. Moreover, electrochemical sensors are more environmentally friendly since they often involve fewer reagents and waste generation [31]. Their ability to be miniaturized and integrated into point-of-care devices further enhances their practicality for widespread applications [32]. As a result, electrochemical sensors are gaining significant attention as a reliable and efficient tool for pharmaceutical determination, addressing many of the limitations posed by traditional methods [33]. However, the first step in the development of a new electrochemical sensor or an adsorptive removal system is finding a material that has a good interaction with the target molecule.

The $C_8B_6N_6$ nanocluster, a fullerene-like structure, exhibits remarkable properties that make it a promising material for adsorption and sensing applications [34]. Its unique composition, consisting of carbon (C), boron (B), and nitrogen (N) atoms, imparts it with a high degree of chemical stability and tunable electronic properties [35]. The presence of boron and nitrogen atoms introduces polar sites within the structure, enhancing its ability to interact with various molecules through dipole-dipole interactions, hydrogen bonding, or van

der Waals forces [36]. This feature is particularly advantageous for adsorption processes, as it allows the nanocluster to effectively capture and hold diverse chemical species [37]. Furthermore, the high surface area of the $C_8B_6N_6$ nanocluster, due to its hollow, cage-like geometry, provides ample active sites for molecular interactions, making it an efficient adsorbent [38]. However, there are certain advantages associated with the $C_8B_6N_6$ nanocluster that also contribute to its functionality as a sensing material [39]. For instance, its electronic structure can be highly sensitive to external perturbations, such as the adsorption of target molecules [40]. Density Functional Theory (DFT) is a powerful and widely used computational quantum mechanical modeling method that has revolutionized the study of electronic structure in materials and molecules [41]. One of its most significant advantages lies in its ability to deliver accurate predictions of the electronic properties of complex systems while remaining computationally efficient compared to other quantum mechanical methods, such as wavefunction-based approaches [42]. This efficiency makes DFT particularly valuable for exploring the adsorption systems of nanostructures, where the interactions between adsorbates and surfaces play a critical role in determining functionality [43]. By employing advanced exchange-correlation functionals, DFT can effectively capture the electronic interactions and binding energies that govern adsorption processes [44]. Furthermore, its flexibility allows researchers to model a wide range of nanostructured materials, including metals, semiconductors, oxides, and 2D materials like graphene or transition metal dichalcogenides [45]. The predictive power of DFT has opened up immense potential for designing and optimizing nanostructures for applications in catalysis, energy storage, sensors, and environmental remediation [46]. For instance, it enables the identification of active sites on catalytic surfaces and provides insights into reaction mechanisms at the atomic level [47]. Additionally, DFT can be combined with machine learning techniques to accelerate the discovery of novel materials with tailored properties [48]. Despite some limitations, such as challenges in accurately describing long-range dispersion interactions or strongly correlated systems, ongoing advancements in computational algorithms and hybrid functionals continue to enhance its accuracy and applicability [49]. Overall, DFT stands as an indispensable tool in modern materials science, offering unparalleled opportunities for understanding and engineering adsorption phenomena in nanostructures [50]. To the best of our knowledge, no prior work has systematically explored the adsorption characteristics of CH on the surface of a $C_8B_6N_6$ nanocluster using DFT methods. This gap in the literature highlights the need for a detailed investigation into the structural and electronic changes that occur during the adsorption process, as well as the thermodynamic feasibility of such interactions. In summary, this study represents a significant step forward in exploring the adsorption behavior of CH on $C_8B_6N_6$ nanoclusters through a DFT-based approach. The findings presented herein will not only enhance our fundamental understanding of molecular-nanocluster interactions but also provide valuable insights for future research and technological applications involving boron nitride-based materials.

Computational Details

In this study, the adsorption of chloral hydrate on the surface of the $C_8B_6N_6$ nanocluster was investigated using Density Functional Theory (DFT) to provide a comprehensive understanding of the interaction mechanisms and associated electronic properties. All computational work was carried out using the Gaussian 16 software package [51], with molecular structure visualization and pre-optimization performed using GaussView 6 [52]. The geometry optimization of the nanocluster and its complexes with chloral hydrate was conducted using the B3LYP [53] hybrid functional, a widely accepted functional for studying molecular systems due to its balanced treatment of exchange and correlation effects. The 6-31G* [54] basis set was employed throughout the study, as it provides a reliable level of accuracy for molecular systems while maintaining computational efficiency. Convergence criteria were carefully monitored to ensure that optimized geometries corresponded to true minima on the potential energy surface, as confirmed by the absence of imaginary frequencies in subsequent frequency calculations. Frequency calculations were performed to evaluate the vibrational modes of the optimized structures and to verify the thermodynamic stability of the adsorption complexes. Infrared (IR) spectra were also simulated to gain insights into potential changes in vibrational characteristics upon adsorption. Thermodynamic parameters,

including Gibbs free energy (ΔG_{ad}), enthalpy (ΔH_{ad}), thermodynamic equilibrium constant (K_{th}) and entropy (ΔS_{ad}), were calculated to evaluate the feasibility and spontaneity of the adsorption process under standard conditions. To further probe the electronic interactions between chloral hydrate and the $C_8B_6N_6$ nanocluster, frontier molecular orbital (FMO) analysis was conducted. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies were calculated to determine the energy gap (E_g), which provides insights into the electronic stability and reactivity of the system. The density of states (DOS) spectra were analyzed using GaussSum 3 software [55] to visualize the contributions of individual molecular orbitals to the overall electronic structure. Overall, this computational approach allowed for a detailed investigation of the structural, electronic, vibrational, and thermodynamic properties of chloral hydrate adsorption on the $C_8B_6N_6$ nanocluster. The results provide valuable insights into the potential applications of boron nitride-based nanoclusters in adsorption and sensor technologies. To account for environmental effects, single-point energy calculations were conducted using the Polarizable Continuum Model (PCM) [56] with water as the solvent. This approach provides insights into adsorption behavior under realistic conditions. The self-consistent field (SCF) calculations were carried out with a convergence criterion of 10^{-6} Hartree for the total electronic energy. This stringent criterion ensures accurate electronic structure calculations and reliable energy differences between adsorption configurations. To improve convergence, the DIIS (Direct Inversion in the Iterative Subspace) algorithm was used, and initial guesses for molecular orbitals were obtained using the Harris functional. To validate the computational approach, benchmark calculations were carried out by comparing the adsorption energies of a test molecule on a similar nanocluster with available experimental or high-level theoretical data. The results confirmed that the chosen methodology provides reliable predictions within acceptable error margins.

RESULTS AND DISCUSSION

Structural and NBO Analysis

The initial and optimized structures depicted in Fig. 1 clearly illustrate the interaction between the CH molecule and the $C_8B_6N_6$ nanocluster, which has been analyzed in three distinct configurations to identify the most stable conformer. In the

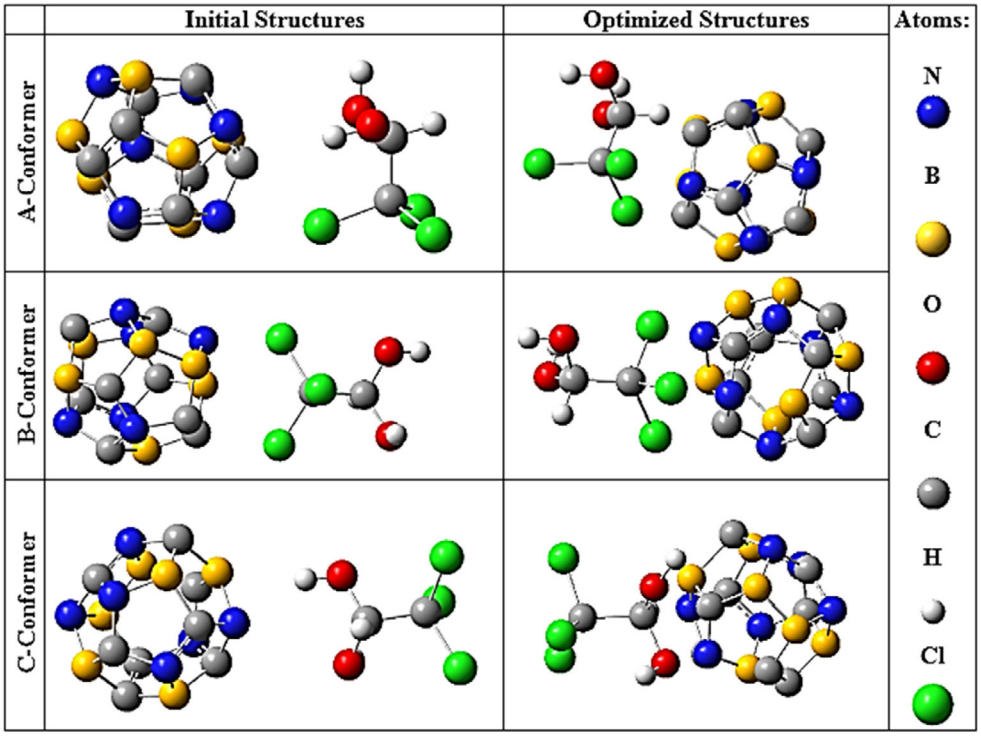

Fig. 1. The initial and optimized structures of CH and $C_8B_6N_6$ complexes

Table 1. Structural properties of CH, $C_8B_6N_6$ and their complexes

Structures	Total electronic energy (a. u.)	Adsorption energy (kJ/mol)	Zero-point energy (kJ/mol)	ν_{min} (cm^{-1})	ν_{max} (cm^{-1})	Dipole moment (Debye)
CH (Vacuum)	-988.771	---	725.516	67.614	4244.939	1.890
CH (Water)	-986.571	---	727.811	67.855	4343.124	2.120
$C_8B_6N_6$ (Vacuum)	-1120.121	---	309.342	398.481	1666.880	0.000
$C_8B_6N_6$ (Water)	-1121.228	---	318.808	399.865	1663.231	0.020
A-Conformer (Vacuum)	-2108.912	-52.510	1121.955	43.820	3793.852	5.969
A-Conformer (Water)	-2107.807	-21.004	1126.655	45.539	3794.492	6.599
B-Conformer (Vacuum)	-2108.931	-102.395	1138.622	36.958	4247.733	7.609
B-Conformer (Water)	-2107.819	-52.510	1123.309	37.797	4249.980	8.579
C-Conformer (Vacuum)	-2108.923	-81.391	1127.809	37.181	4332.898	9.499
C-Conformer (Water)	-2107.812	-34.132	1132.111	39.650	4334.968	10.469

A-Conformer, the CH molecule is oriented parallel to the nanocluster, positioned adjacent to its side chlorine and hydrogen atoms. In the B-Conformer, the CH molecule is situated near the $C_8B_6N_6$ nanocluster, with its chlorine atoms directed towards the cluster. Lastly, in the C-Conformer, the CH molecule is positioned close to the nanocage, oriented towards its OH groups. As illustrated in Fig. 1, both the initial and optimized structures demonstrate that no significant structural distortions have occurred during the geometrical optimization process [57]. Therefore, the interactions appear to be relatively weak, suggesting that a physisorption mechanism predominates across all configurations [58]. The results obtained are summarized in Table 1. As observed, the total electronic energy of the B-Conformer is more negative compared to the A and C configurations [59]. This indicates that the interactions within the B-Conformer are stronger, making its formation more experimentally favorable. The calculated adsorption energies are summarized in Table 1. As evident, all the obtained adsorption energies for the three different conformers are negative, indicating that the adsorption process is experimentally feasible [60]. Among them, the adsorption energy of the B-Conformer is lower compared to those of the A and C configurations, suggesting that the formation of the B-Conformer is energetically more favorable than the others [61]. The effect of water as a solvent was also examined using the PCM solvation method. The results, presented in Table 1, reveal that while the adsorption energy values slightly decrease in the aqueous phase, they remain negative [62]. This observation suggests that the adsorption process is still experimentally feasible in the aqueous phase, although the interactions are somewhat weaker compared to those in the gaseous phase [63].

The adsorption energy values for all examined conformers, in both gaseous and aqueous phases, are below 150 kJ/mol, suggesting that the adsorption mechanism is likely physisorption [64]. To gain deeper insights into the adsorption mechanism, natural bond orbital (NBO) calculations were performed on the optimized structures [65]. The results confirmed the absence of any bond formation between the adsorbate and the adsorbent, further validating that the adsorption mechanism is definitively physisorption [66]. Following the geometrical optimization, IR calculations were performed on all evaluated structures. The maximum and minimum calculated IR frequencies are presented in Table 1. As observed, no negative values were obtained, indicating that all the analyzed structures represent true local minima [67].

Thermodynamic Parameters

The thermodynamic parameters calculated for the study are summarized in Table 2. The data clearly indicate that the adsorption process is highly exothermic and spontaneous. This conclusion is supported by the consistently negative values of both ΔH_{ad} and ΔG_{ad} across all three conformers, regardless of whether the process occurs in the aqueous or gaseous phase. These negative values signify that the adsorption releases energy (exothermic nature) and proceeds without the need for external input (spontaneity) [68]. The values of K_{th} suggest that the interactions are reversible and exist in a state of equilibrium, indicating a dynamic balance between adsorption and desorption processes [69]. The negative values of ΔS_{ad} imply that the interactions are not favorable from an entropy perspective, likely due

Table 2. The calculated thermodynamic parameters in 298-318 K at 10° intervals

NO	ΔH_{ad} (kJ/mol)	ΔG_{ad} (kJ/mol)	ΔS_{ad} (J/mol)	K_{th}
A-Conformer-Vacuum-298	-63.381	-65.812	-141.891	$3.392\times10^{+11}$
A-Conformer-Vacuum-308	-61.040	-63.471	-144.450	$5.746\times10^{+10}$
A-Conformer-Vacuum-318	-58.699	-61.130	-147.012	$1.089\times10^{+10}$
A-Conformer-Water-298	-31.875	-34.306	-136.103	$1.024\times10^{+06}$
A-Conformer-Water-308	-29.534	-31.965	-138.665	$2.622\times10^{+05}$
A-Conformer-Water-318	-27.193	-29.624	-142.221	$7.310\times10^{+04}$
B-Conformer-Vacuum-298	-113.266	-115.697	-123.699	$1.864\times10^{+20}$
B-Conformer-Vacuum-308	-110.925	-113.356	-126.260	$1.643\times10^{+19}$
B-Conformer-Vacuum-318	-108.584	-111.015	-128.828	$1.688\times10^{+18}$
B-Conformer-Water-298	-63.381	-65.812	-134.212	$3.392\times10^{+11}$
B-Conformer-Water-308	-61.040	-63.471	-132.069	$5.746\times10^{+10}$
B-Conformer-Water-318	-58.699	-61.130	-134.638	$1.089\times10^{+10}$
C-Conformer-Vacuum-298	-92.262	-94.693	-136.743	$3.894\times10^{+16}$
C-Conformer-Vacuum-308	-89.921	-92.352	-139.302	$4.521\times10^{+15}$
C-Conformer-Vacuum-318	-87.580	-90.011	-141.868	$6.008\times10^{+14}$
C-Conformer-Water-298	-45.003	-47.434	-129.889	$2.044\times10^{+08}$
C-Conformer-Water-308	-42.662	-45.093	-132.456	$4.406\times10^{+07}$
C-Conformer-Water-318	-40.321	-42.752	-135.015	$1.046\times10^{+07}$

to the aggregation of nanoclusters following the adsorption process [70]. This aggregation reduces the system's disorder, thereby contributing to the unfavorable entropy change. The influence of temperature on all thermodynamic parameters was thoroughly examined. The findings reveal that as the temperature increases, both ΔH_{ad} (enthalpy change) and ΔG_{ad} (Gibbs free energy change) become more positive [71]. This suggests that the adsorption process becomes less thermodynamically favorable with rising temperature. On the other hand, the values of ΔSad (entropy change) and K_{th} (equilibrium constant) decrease as temperature increases, further indicating that the interactions are more energetically and entropically favorable at lower temperatures [72]. This behavior highlights that lower temperatures promote stronger and more stable interactions, while higher temperatures disrupt the equilibrium, making the adsorption process less efficient [73].

FMO Analysis

The examination of frontier molecular orbital (FMO) parameters, as detailed in Table 3 and Fig. 3, reveals significant changes in the band gap of $C_8B_6N_6$ upon adsorption. Initially measured at 2.178 eV, the band gap decreases markedly to 1.392 eV, 1.046 eV, and 1.315 eV for conformers A, B, and C, respectively. This represents a substantial maximum reduction of approximately 51.997% for the most favorable conformer. Such a dramatic decline in the band gap highlights the remarkable potential of $C_8B_6N_6$ as an effective electrocatalyst modifier, particularly for detecting CH molecules [74]. The decrease in the band gap indicates an enhanced electronic interaction between $C_8B_6N_6$ and the adsorbed species, which could lead to improved charge transfer properties [75]. This is a crucial characteristic for materials used in electrocatalysis, as it directly impacts their sensitivity and efficiency in detecting specific molecules [76]. The variation in band gap values across different conformers suggests that the structural configuration of $C_8B_6N_6$ plays a pivotal role in its electronic properties and interaction with adsorbates. The results underscore the adaptability of $C_8B_6N_6$ as a tunable material, with conformer B showing the most significant reduction in band gap [77]. This makes it particularly promising for applications requiring precise and efficient molecular detection. The findings pave the way for further exploration of $C_8B_6N_6$ in advanced sensor technologies and electrocatalytic systems, where its ability to modify electronic properties upon interaction with target molecules could be harnessed for innovative solutions in chemical sensing and energy applications [78]. The adsorption process leads to a noticeable decrease in the chemical hardness of CH, reducing it from its initial value of 3.472 eV to 0.696 eV, 0.523 eV, and 0.657 eV for the respective conformers. This reduction in chemical hardness signifies an

Table 3. The computed FMO parameters

Structures	E_{HOMO} (eV)	E_{LUMO} (eV)	Eg (eV)	%ΔEg	η (eV)	μ (eV)	ω (eV)	ΔN_{max} (eV)
CH	-8.390	-1.446	6.944	---	3.472	-4.918	3.484	1.417
$C_8B_6N_6$	-5.750	-3.572	2.178	---	1.089	-4.661	9.973	4.280
A-Conformer	-4.830	-3.438	1.392	-36.098	0.696	-4.134	12.279	5.940
B-Conformer	-4.155	-3.109	1.046	-51.977	0.523	-3.632	12.614	6.945
C-Conformer	-4.788	-3.473	1.315	-39.631	0.657	-4.130	12.973	6.282

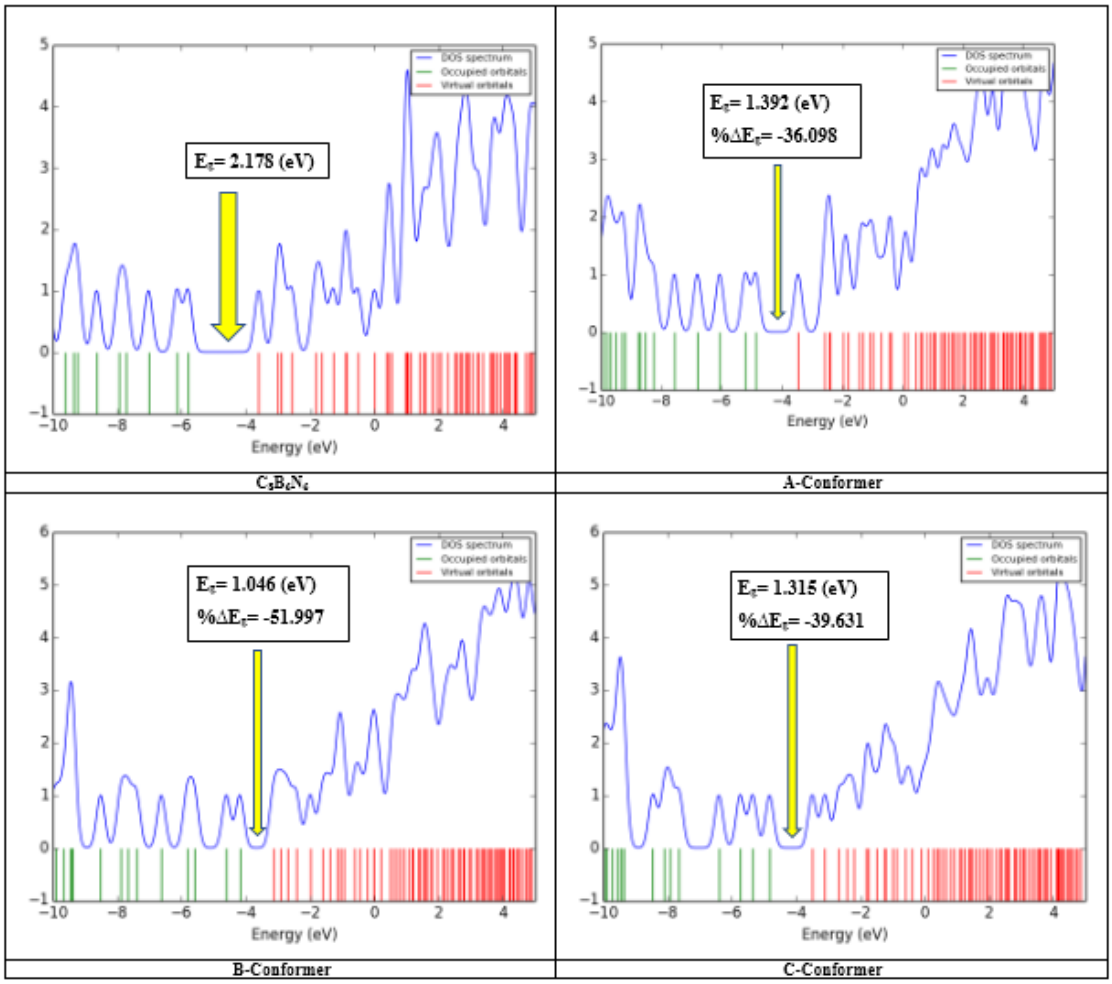

Fig. 2. The computed DOS spectrums

increase in chemical reactivity after adsorption, as lower chemical hardness typically correlates with a greater tendency to participate in chemical reactions [79]. Moreover, the negative values of chemical potential observed in these configurations provide further evidence of their thermodynamic stability. These findings indicate that the adsorption process not only enhances the chemical reactivity of CH but also significantly stabilizes the resulting conformers [80]. This stabilization makes these conformers more favorable for practical applications in a wide range of chemical and material systems [81-83]. Furthermore, the process of adsorption leads to notable increases in both the electrophilicity index and the maximum charge transfer capacity for CH when adsorbed onto the $C_8B_6N_6$ surface. This suggests that the interaction with the nanostructured surface substantially boosts CH's ability to absorb electrons, a capability that is markedly reduced in isolated CH molecules without such interactions [84]. These insights highlight the transformative role of adsorption in

improving the electronic properties and functional potential of CH, opening up new avenues for its use in advanced material design, catalysis, and other technological applications.

CONCLUSION

In this work, the adsorption behavior of chloral hydrate (CH) on a $C_8B_6N_6$ fullerene-like nanocluster was comprehensively investigated using Density Functional Theory calculations. Three different adsorption configurations were examined in both gaseous and aqueous phases to determine the most stable interaction mode. The calculated adsorption energies were negative for all conformers, confirming the thermodynamic feasibility of the adsorption process. Among the studied configurations, the B-conformer exhibited the strongest interaction and highest stability, making it the most favorable adsorption structure. The magnitude of adsorption energies (below 150 kJ/mol), absence of new bond formation from NBO analysis, and negligible structural distortions collectively indicate that the adsorption mechanism is predominantly physisorption. Solvent effects slightly weakened the interactions but did not alter the spontaneous nature of the process. Thermodynamic parameters further confirmed that the adsorption is exothermic and spontaneous across the investigated temperature range (298–318 K), with lower temperatures favoring stronger adsorption. The negative entropy changes suggest increased order upon adsorption, consistent with adsorbate–adsorbent association. Frontier molecular orbital analysis revealed a significant reduction in the band gap of $C_8B_6N_6$ after CH adsorption, particularly for the B-conformer, indicating enhanced electronic sensitivity and charge transfer characteristics. The decrease in chemical hardness and increase in electrophilicity and maximum charge transfer capacity further demonstrate that adsorption substantially modifies the electronic properties of the nanocluster. These electronic changes highlight the strong potential of $C_8B_6N_6$ as a sensing material for chloral hydrate detection. Overall, this theoretical study provides valuable molecular-level insight into the interaction mechanism between CH and $C_8B_6N_6$ nanoclusters. The results suggest that $C_8B_6N_6$ is a promising candidate for chloral hydrate adsorption and sensor development, particularly in environmental monitoring applications. Future experimental validation and exploration of functionalized derivatives may further enhance their practical applicability.

CONFLICT OF INTEREST STATEMENT

The authors declare that there are no conflicts of interest related to the research, authorship, or publication of this manuscript. All authors have disclosed any financial or personal relationships that could potentially influence or bias the work presented.

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