

Structural and Electronic Properties of Chloroform-Adsorbed GaN Nanosheet-Like Clusters: A First-Principles Study

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Abstract: The present study aims to investigate the adsorption behavior of chloroform (CHCl_3) on a gallium nitride nanosheet (GaNNS) cluster and evaluate its potential application as a sensing material for CHCl_3 detection. Dispersion-corrected density functional theory (DFT-D) calculations were performed using the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional, as implemented in the DMol³ module of Materials Studio. Two adsorption structures were optimized from initially hydrogen-facing and chlorine-facing orientations. Both relaxed configurations exhibited $\text{H}\cdots\text{N}$ contacts, with distances of 2.040 and 2.219 Å, respectively. The calculated adsorption energies were -0.614 and -0.620 eV, respectively, revealing favorable adsorption with a negligible energetic distinction between the two starting orientations. Hirshfeld analysis yields net CHCl_3 fragment charges of $+0.0498$ and $+0.0268$ e, consistent with weak electron redistribution from the molecule toward the GaNNS framework. The calculated HOMO–LUMO gap increases from 0.348 eV for isolated GaNNS to 0.508 and 0.509 eV for the adsorption complexes. Total and projected density-of-states analyses further illustrate adsorption-associated changes in the electronic-state distribution. Together, the moderate adsorption energies, noncovalent $\text{H}\cdots\text{N}$ contacts, and limited charge redistribution favor a predominantly physisorption-like interaction with an electronic contribution. The adsorption-induced electronic response identifies GaNNS-based nanostructures as candidates for CHCl_3 sensing.

Keywords: Gallium Nitride; Chloroform; Density Functional Theory; Adsorption; Hirshfeld Charge; HOMO–LUMO; Density of States.

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I. INTRODUCTION

Detection of volatile organic compounds is important in environmental monitoring and industrial safety [1,2]. Chloroform (CHCl_3), a chlorinated volatile compound, is particularly relevant because its presence in air or process streams motivates sensitive detection strategies [3]. At the molecular level, an effective sensing surface must interact sufficiently with the analyte to produce a measurable response while retaining the possibility of analyte release. Atomistic calculations provide a route to examine this balance through adsorption energetics, interfacial geometry, charge redistribution, and electronic-structure changes.

Since the discovery of graphene, two-dimensional (2D) nanomaterials have garnered considerable research interest owing to their unique electronic and optical properties [4]. Previous studies have demonstrated that two-dimensional (2D) hexagonal semiconductors exhibit superior electronic and

physical properties compared with their bulk counterparts [5,6]. In particular, graphene has emerged as a promising material for gas-sensing applications owing to its large specific surface area, high surface-to-volume ratio, and excellent charge-carrier mobility [7]. Among the wide range of promising nanomaterials [8-10], Low-dimensional GaNNS has attracted theoretical interest because its polar Ga–N framework offers chemically distinct adsorption environments [11-13]. Prior DFT-D work by Roohi and Askari Ardehjani examined SO_2 and NO_2 adsorption on pristine and transition-metal-doped GaNNS and demonstrated how adsorption energies, charge-transfer analyses, and electronic gaps can be considered together when screening candidate gas-sensitive materials [14]. These observations motivate investigating chlorinated molecules on GaNNS structures.

Adsorption can be discussed in terms of physisorption and chemisorption. Physisorption is generally associated with dispersion, electrostatic interactions, and weak intermolecular

contacts, whereas chemisorption involves appreciable chemical-bond formation and orbital reorganization [15]. Adsorption energy alone does not impose a universal boundary between these regimes; a sound interpretation also considers relaxed geometry, charge distribution, and electronic structure. Likewise, a change in the frontier-orbital separation can indicate an electronic response, but is not itself a measured sensor signal.

Here, dispersion-corrected DFT calculations are used to explore the interaction between CHCl_3 and a GaNNS like cluster. We compare two initial molecular orientations and relate their optimized adsorption structures to energetic stability, Hirshfeld charges, frontier orbitals, and total/projected density of states. The objective is to establish a coherent microscopic picture of adsorption and evaluate whether the calculated response warrants further exploration of GaNNS-based CHCl_3 sensing.

II. COMPUTATIONAL METHODOLOGY

The GaN model consists of nine gallium and nine nitrogen atoms arranged as a finite nanosheet of Ga_9N_9 cluster (18 atoms). The isolated CHCl_3 molecule contains one C, one H, and three Cl atoms, giving 23 atoms in each adsorption complex. The GaNNS and CHCl_3 molecule were optimized separately. Adsorption models were then assembled with the hydrogen or chlorine side of CHCl_3 initially directed toward the GaN framework; each was fully relaxed. The H-facing and Cl-facing descriptors therefore denote the starting orientations, not necessarily distinct final chemical bonding motifs.

Electronic-structure calculations were performed with the DMol³ module of Materials Studio [16], using the generalized-gradient approximation of Perdew, Burke, and Ernzerhof (PBE) [17], a double-numerical-plus-polarization (DNP) basis, Fine calculation quality, and a Tkatchenko–Scheffler dispersion correction [18]. The reported calculations used neutral systems and no symmetry constraints. Dispersion correction is pertinent because weak intermolecular forces may contribute substantially to CHCl_3 adsorption. The structural model was treated as a finite cluster rather than a periodic slab. The adsorption energy was calculated from the dispersion-corrected total energies using:

$$E_{\text{ads}} = E_{\text{GaNNS}+\text{CHCl}_3} - E_{\text{GaNNS}} - E_{\text{CHCl}_3}$$

Here, $E_{\text{GaNNS}+\text{CHCl}_3}$ is the total energy of the optimized adsorption complex, while the remaining terms represent the optimized isolated components calculated with comparable settings. Negative E_{ads} indicates that the optimized combined configuration is lower in energy than the selected isolated-component reference. The reported values do not include a zero-point energy, entropy, temperature correction, or counterpoise basis-set superposition error correction.

The frontier-orbital separation was calculated as Band gap = $(E_{\text{LUMO}} - E_{\text{HOMO}}) \times 27.2114 \text{ eV Ha}^{-1}$. For a finite cluster this is a Kohn–Sham molecular-orbital gap. Hirshfeld charges were assigned to atoms and summed over the CHCl_3 fragment to obtain its net charge [19]. Total and orbital-projected densities of states (DOS and PDOS) were examined for the isolated components and adsorption complexes. For finite GaNNS, DOS plots are broadened distributions of discrete molecular levels; peak positions and magnitudes depend on broadening and energy referencing.

III. RESULTS AND DISCUSSION

➤ Structural Models and Adsorption Geometry

The optimized isolated molecule and the top and side views of the GaNNS framework are presented in Figure 1. The alternating Ga and N sites provide a polar adsorption environment, while the finite geometry preserves a compact surface-like arrangement. As illustrated in Figure 1(b, c), the optimized GaNNS exhibits a hexagonal framework consisting of alternating Ga and N atoms. Owing to its finite dimensions, several edge atoms remain under coordinated, potentially giving rise to unsaturated dangling bonds and localized electronic states. Furthermore, slight deviations from the ideal hexagonal arrangement are observed, suggesting local structural relaxation within the Ga–N framework [20]. These under coordinated edge sites may provide favorable interaction centers for CHCl_3 adsorption by facilitating local polarization and intermolecular interactions. Consequently, the structural characteristics of the GaNNS are expected to play an important role in determining its adsorption behavior and electronic response toward CHCl_3 .

Figure 2 compares the two starting orientations with their relaxed structures. After optimization, both arrangements display an $\text{H}\cdots\text{N}$ contact between the chloroform hydrogen and a nitrogen atom of the cluster. The corresponding distances are 2.040 Å for the initially H-facing structure and 2.219 Å for the initially Cl-facing structure. The 0.179 Å difference indicates a closer local approach in the former case, although local separation alone is not a measure of total adsorption stability. The relaxation of the Cl-facing starting geometry toward an $\text{H}\cdots\text{N}$ interaction is especially informative: the molecule responds to the local polar environment rather than preserving its original orientation.

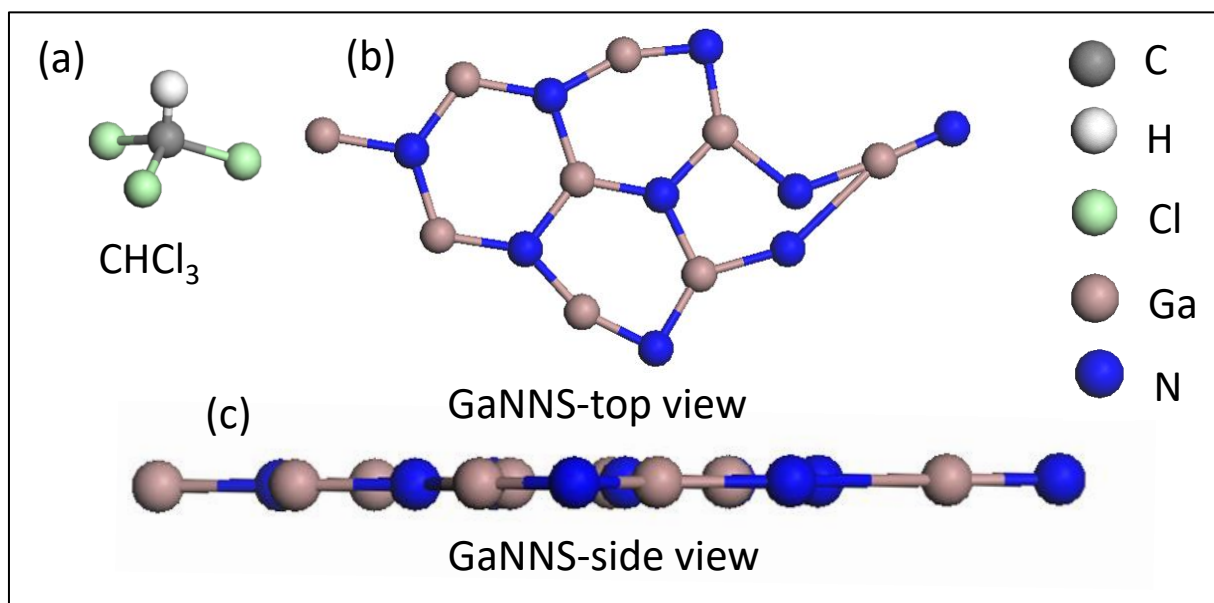


Fig 1 Optimized Structural Models: (a) Isolated CHCl_3 Molecule, (b) Top View of the GaNNS, and (c) Side View of the GaNNS. Atom Colors Follow the Element Key Displayed in the Figure (C, H, Ga, Cl, and N).

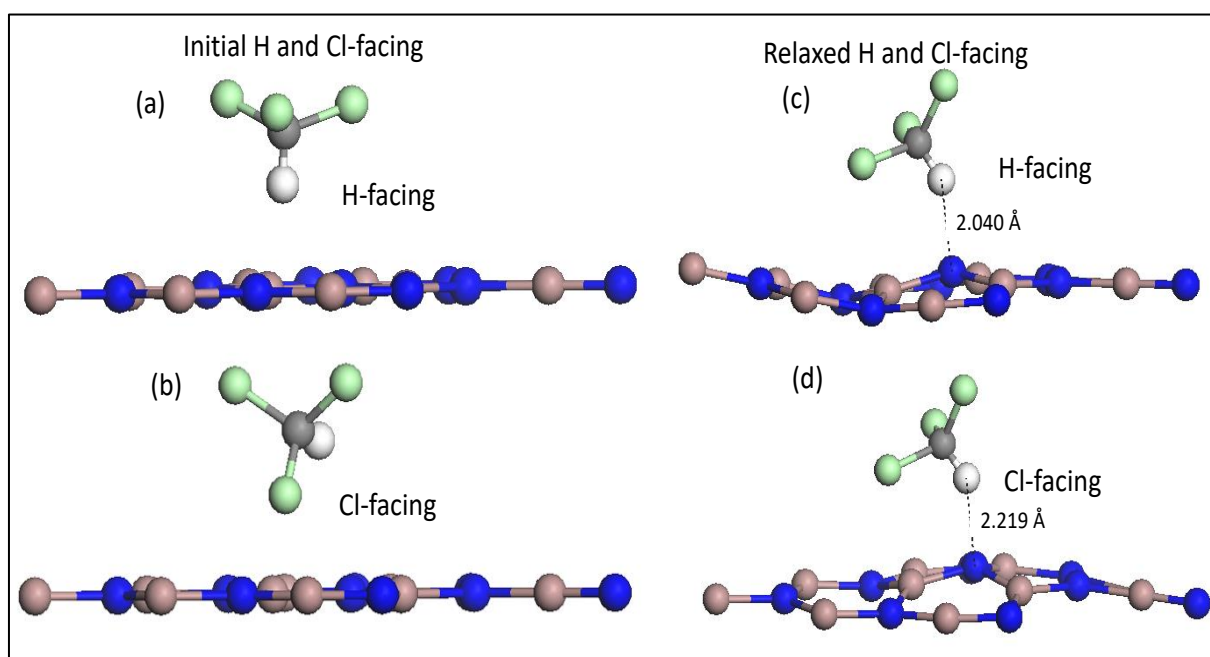


Fig 2 Initial and optimized configurations of CHCl_3 on GANNS: (a) initial H-facing arrangement; (b) initial Cl-facing arrangement; (c) relaxed structure originating from the H-facing arrangement, showing an $\text{H}\cdots\text{N}$ contact of 2.040 Å; and (d) relaxed structure originating from the Cl-facing arrangement, showing an $\text{H}\cdots\text{N}$ contact of 2.219 Å.

➤ Adsorption Energetics and Configuration Comparison

The calculated adsorption energies are -0.614 eV for the initially H-facing complex and -0.620 eV for the initially Cl-facing complex (Table 1). Both negative values show that the relaxed adsorbate-cluster arrangements are energetically favored over the separated components which can be compared with previous report [21]. The difference is only 0.005 eV at the tabulated precision, indicating essentially comparable adsorption stability. In fact, the Cl-facing starting arrangement relaxes to an $\text{H}\cdots\text{N}$ -contact geometry and has a slightly more negative adsorption energy despite its longer measured $\text{H}\cdots\text{N}$ distance. This contrast emphasizes that the adsorption energy reflects the entire molecule-cluster interaction, including

dispersion and electrostatic contributions, rather than a single interatomic distance.

The combination of moderately negative adsorption energies, retained molecular identity, $\text{H}\cdots\text{N}$ intermolecular contacts, and small net charge redistribution is most consistent with predominantly physisorption-like adsorption accompanied by interfacial polarization. The present data do not demonstrate formation of a new covalent Ga-Cl, Ga-C, or N-H bond, so describing the interaction as established chemisorption would be stronger than the evidence supports.

At the same time, the adsorption is not electronically inert: the electronic response discussed below suggests coupling between the molecule and the GaN framework. Such an adsorption regime is of interest for sensing concepts because reversible molecular interaction and measurable electronic perturbation are both desirable characteristics.

➤ Hirshfeld Charge Redistribution

Hirshfeld population analysis (Figure 3) provides a complementary view of the adsorption interaction. The net charges assigned to CHCl_3 are +0.0498 e in the initially H-facing complex and +0.0268 e in the initially Cl-facing

complex. Their positive signs indicate that the adsorbate becomes slightly electron deficient under the Hirshfeld partitioning scheme, corresponding to a small net electron redistribution toward GaNNS. The H-facing geometry exhibits the larger redistribution, which is consistent with its shorter $\text{H}\cdots\text{N}$ contact. The magnitudes remain modest, however, supporting a weakly polarized adsorbate–surface interface rather than extensive electron transfer. These charges depend on the selected population-analysis method and should be understood as a comparative descriptor of the calculated electron density.

Table 1 Comparison of the Calculated Total Energies, Adsorption Energies (E_{ads}), Frontier-Orbital Energies, HOMO–LUMO Gaps, and Hirshfeld Fragment Charges for GaNNS, Isolated CHCl_3 , and the Two Optimized Adsorption Complexes.

Parameters	GaNNS	CHCl_3	H-facing	Cl-facing
Number of atoms	18	5	23	23
Total energy (Ha)	-17814.0321	-1418.7731	-19232.82776	-19232.82797
E_{ads} (eV)	—	—	-0.614	-0.620
HOMO energy (Ha)	-0.180	-0.271	-0.180	-0.181
LUMO energy (Ha)	-0.167	-0.077	-0.161	-0.162
HOMO–LUMO gap (eV)	0.348	5.269	0.508	0.509
Hirshfeld charge on CHCl_3 (e)	—	0	0.050	0.027

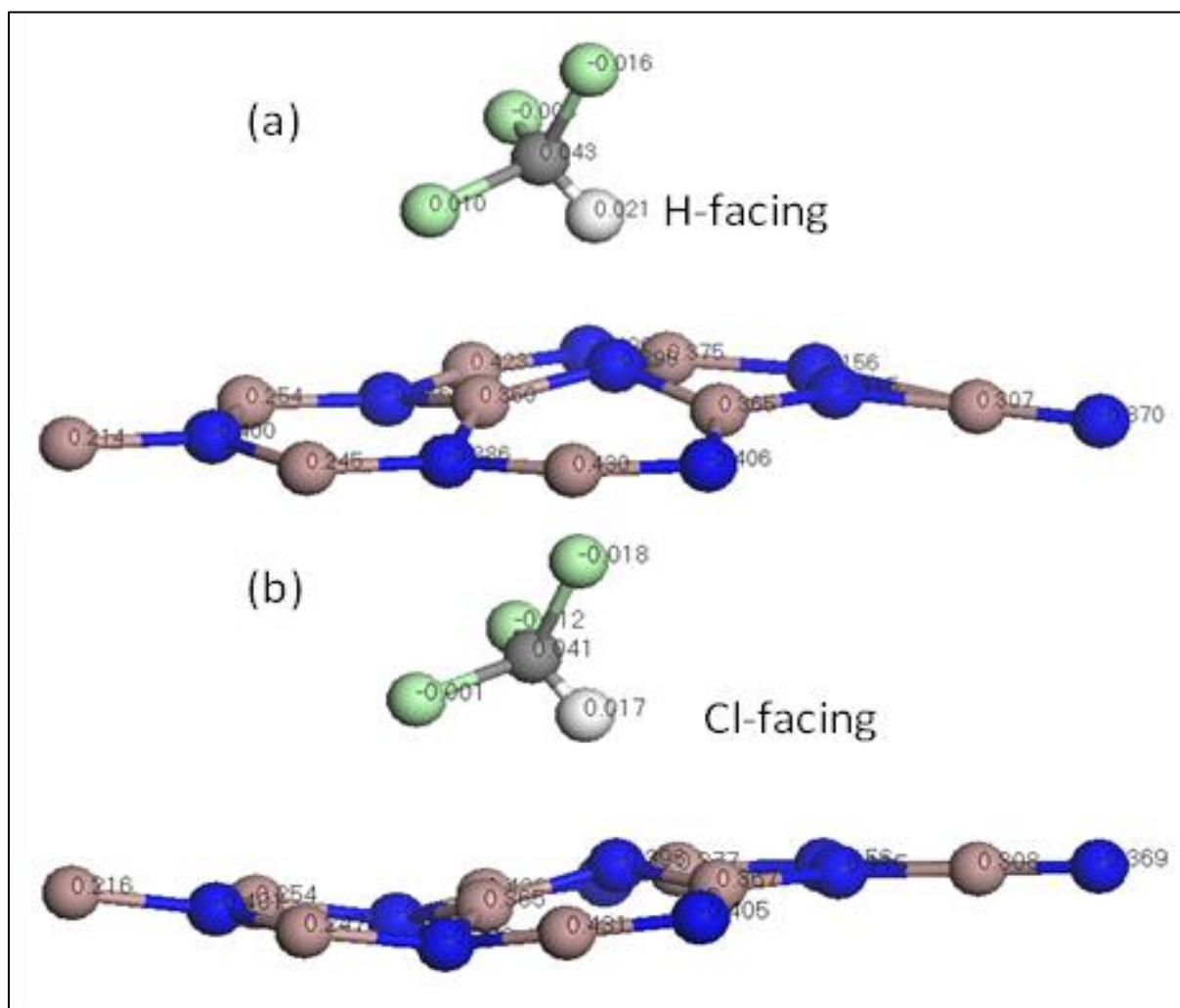


Fig 3 Hirshfeld atomic-charge distributions of the optimized adsorption complexes: (a) initially H-facing configuration and (b) initially Cl-facing configuration. The net Hirshfeld charges assigned to the CHCl_3 fragment are +0.0498 e and +0.0268 e, respectively; the displayed atom labels are partial charges.

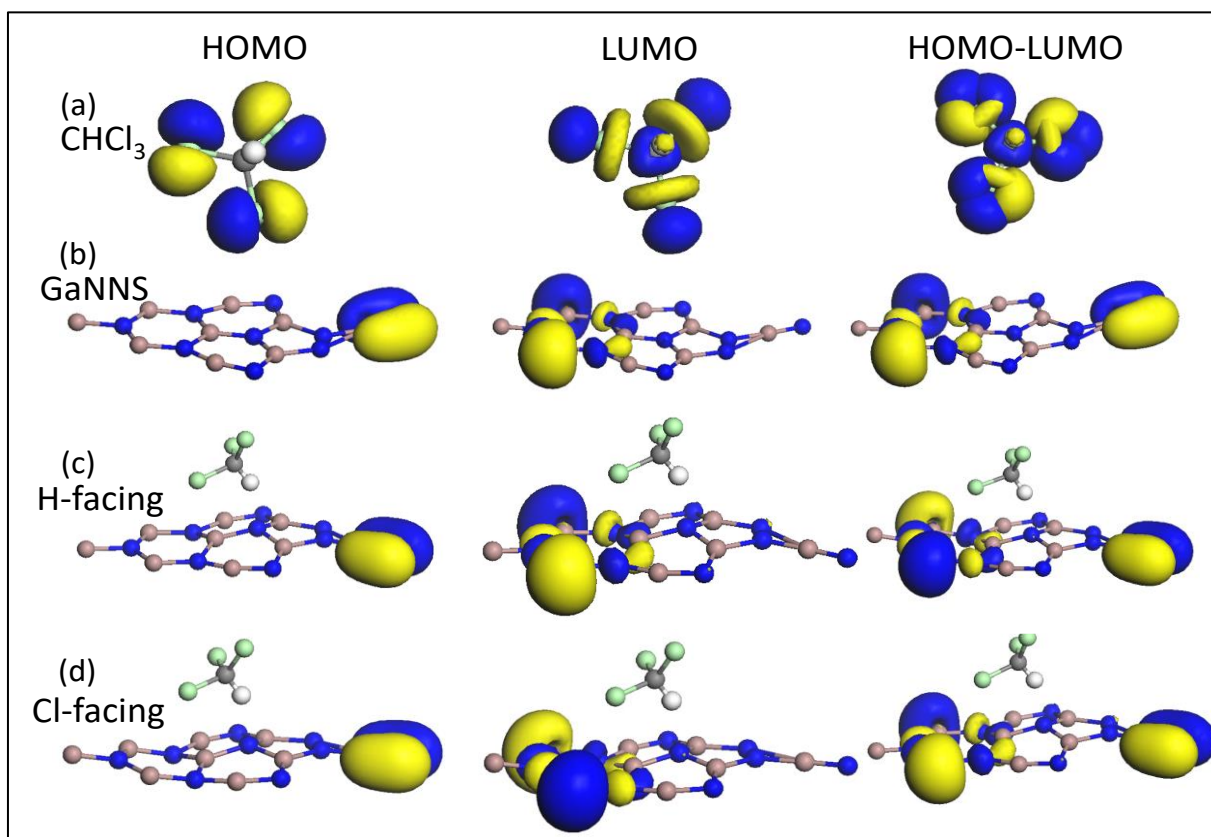


Fig 4 Frontier molecular-orbital isosurfaces for (a) isolated CHCl_3 , (b) pristine finite GaNNS, (c) the optimized initially H-facing adsorption complex, and (d) the optimized initially Cl-facing adsorption complex. For each row, the displayed orbitals are HOMO and LUMO representations; blue and yellow lobes indicate opposite orbital phases, not positive and negative charges.

➤ Frontier Molecular Orbitals and Energy Gaps

The frontier-orbital analysis (Figure 4 and Table 1) indicates that CHCl_3 adsorption modifies the electronic structure of the GaNNS. The reported HOMO–LUMO gap is 0.348 eV for pristine GaNNS and 5.269 eV for isolated CHCl_3 . Following adsorption, the gaps become 0.508 eV for the initially H-facing complex and 0.509 eV for the initially Cl-facing complex. Thus, relative to the pristine cluster, the gap increases by 0.160 and 0.161 eV, respectively—approximately 46% in each case. This near-identical response is consistent with the similarity of the two relaxed adsorption motifs [21,22]. The larger gap is evidence of an adsorption-associated change in the frontier-level separation; it should not be presented as an experimentally established increase or decrease in electrical conductivity. For a finite cluster, frontier levels may also be influenced by the edge-atom electronic structure.

The HOMO and LUMO isosurfaces in Figure 4 complement the numerical gaps by showing the spatial distribution of the frontier states. Comparing the isolated components with the adsorption complexes helps visualize how molecular proximity perturbs the accessible electronic states. The most defensible interpretation is therefore a combined structural and electronic response: the adsorbate binds favorably, redistributes a small amount of electron density, and changes the cluster's frontier-level spacing. This set of effects supplies a plausible atomistic basis for a detectable electrical or spectroscopic signal in a suitably engineered GaNNS-based sensor.

➤ Total and Projected Density of States

The total density of states (TDOS) and projected density of states (PDOS) were analyzed to investigate the electronic structure of the pristine GaNNS and the modifications induced by CHCl_3 adsorption. As illustrated in Figure 5(a–f), the electronic states exhibit distinct distributions and peak intensities, reflecting the contributions of different atomic orbitals and their response to molecular adsorption [22,23]. The PDOS spectra reveal substantial contributions from p-orbital states, indicating their important role in determining the electronic characteristics of the GaNNS and its interaction with CHCl_3 .

For the pristine GaNNS, the PDOS spectrum exhibits two prominent peaks, designated as p1 and p2, located at approximately -6.62 and -3.39 eV, with corresponding intensities of 14.7 and 14.6 e/eV, respectively. These features represent pronounced contributions from p-orbital states within the GaN electronic structure. Following CHCl_3 adsorption, noticeable changes in the PDOS distribution are observed for both optimized configurations. In the H-facing configuration, a prominent peak (p3) appears at approximately -3.80 eV, with an intensity of 22.0 e/eV. Similarly, the Cl-facing configuration exhibits a characteristic peak (p4) at approximately -3.76 eV, with a corresponding intensity of 21.2 e/eV. The enhanced PDOS peak intensities in the adsorption complexes indicate a redistribution of orbital contributions associated with the interaction between CHCl_3 and the GaNNS. The slightly greater peak intensity in the H-facing configuration suggests a stronger contribution from the projected states within this

energy region, although it does not independently establish a stronger overall adsorption interaction.

Further insights are obtained from the TDOS spectra. The pristine GaN cluster exhibits a characteristic TDOS peak at approximately -3.87 eV, with an intensity of 10.3 eV. Upon CHCl_3 adsorption, the corresponding prominent features occur at approximately -3.77 eV for the H-facing configuration and -3.68 eV for the Cl-facing configuration, with increased intensities of 17.6 and 16.8 eV, respectively. Relative to the pristine cluster, these peak intensities increase by approximately 70.9% and 63.1% for the H-facing and Cl-facing configurations, respectively. These results demonstrate that CHCl_3 adsorption modifies the distribution and spectral weight of the electronic states in the investigated complexes.

The changes in the DOS and PDOS spectra are consistent with the adsorption-induced electronic perturbations indicated by the Hirshfeld charge analysis and frontier molecular orbital calculations. The calculated HOMO–LUMO gap increases from 0.348 eV for the pristine GaN cluster to 0.508 and 0.509 eV for the H-facing and Cl-facing adsorption complexes, respectively. These modifications suggest that the interaction with CHCl_3 affects both the frontier electronic states and the broader electronic-state distribution of the GaNNS. Combined with the favorable adsorption energies of -0.614 and -0.620 eV, the results support predominantly physisorption-like interactions accompanied by electronic polarization and modest charge redistribution, rather than providing conclusive evidence of covalent bond formation.

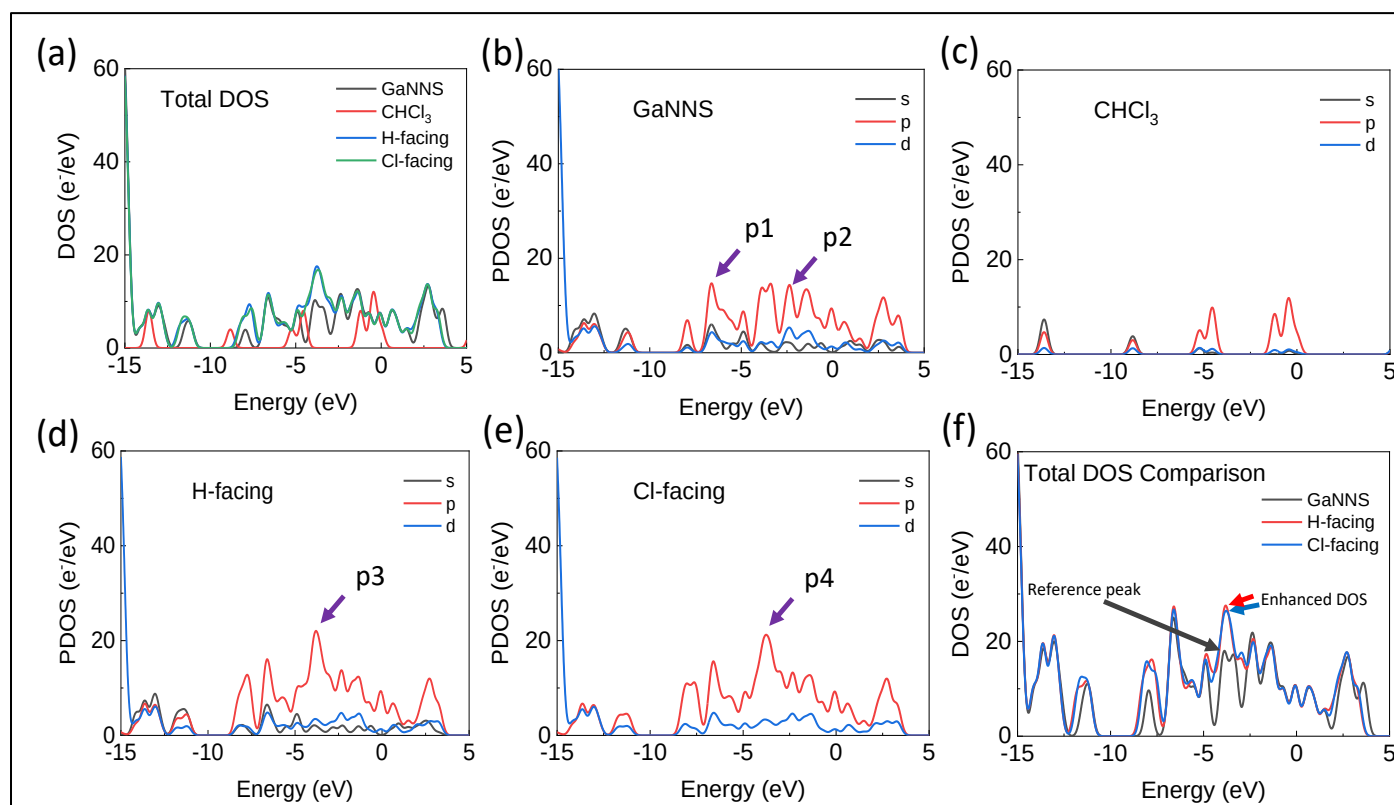


Fig 5 (a) Total density of states (DOS) for pristine GaNNS, isolated CHCl_3 , and the two adsorption complexes; (b) GaNNS projected DOS (PDOS); (c) CHCl_3 PDOS; (d) initially H-facing adsorption-complex PDOS; (e) initially Cl-facing adsorption-complex PDOS; and (f) total-DOS comparison for GaNNS sheet and both complexes. Black, red, and blue curves in panels (b–e) represent s, p, and d contributions, respectively

IV. CONCLUSIONS

Dispersion-corrected DFT calculations reveal favorable adsorption of CHCl_3 on a GaNNS from both H-facing and Cl-facing starting arrangements. The optimized structures show $\text{H}\cdots\text{N}$ contacts of 2.040 and 2.219 Å, while the adsorption energies are -0.614 and -0.620 eV, indicating comparable stability. Hirshfeld analysis identifies modest adsorbate-to-cluster charge redistribution of $+0.0498$ and $+0.0268$ e on CHCl_3 . Adsorption also increases the calculated cluster HOMO–LUMO gap from 0.348 eV to 0.508 – 0.509 eV, accompanied by changes in the DOS/PDOS profiles. Collectively, these observations favor predominantly physisorption-like binding with measurable electronic

perturbation rather than definitive covalent chemisorption. The results suggest that GaN-based nanostructures merit further evaluation as CHCl_3 -responsive sensing platforms. Higher-level calculations on extended and chemically realistic GaN structures, together with experimental adsorption and sensing measurements, can establish whether this predicted molecular-scale response translates into practical sensor operation.

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