Tunable Photocatalytic Properties of Planar GaN/GeC Hetero-Bilayer: Production of H₂ Fuel

MD. SAKIB HASAN KHAN, MD. RAFIQUL ISLAM, (Member, IEEE), MUHAMMAD SHAFFATUL ISLAM, IBRAHIM M. MEHEDI, (Center of Excellence in Intelligent Engineering Systems, King Abdulaziz University, Jeddah 21589, Saudi Arabia) AND MD. TANVIR HASAN, (Member, IEEE)

1Department of Electrical and Electronic Engineering, Khulna University of Engineering & Technology, Khulna 9203, Bangladesh
2Department of Electrical and Electronic Engineering, World University of Bangladesh, Dhaka 1205, Bangladesh
3Department of Electrical and Electronic Engineering, King Abdulaziz University, Jeddah 21589, Saudi Arabia
4Center of Excellence in Intelligent Engineering Systems, King Abdulaziz University, Jeddah 21589, Saudi Arabia
5Department of Electrical and Electronic Engineering, Jashore University of Science and Technology, Jashore 7408, Bangladesh

Corresponding author: Md. Tanvir Hasan (tan_vir_bd@yahoo.com)
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ABSTRACT Novel GaN-based van der Walls (vdW) hetero-bilayer (HBL) is systemically studied through the first-principles density functional theory (DFT) framework to explore its optoelectronic property facilitated photocatalytic activity for hydrogen (H₂) fuel production. The vdW concept of planar GaN with GeC monolayer, together making stacked hetero-bilayer, shows unique and tunable optoelectronic properties that fulfill all the photocatalysis attributes. The confirmation of chemical and dynamical stabilities is made with negative interlayer binding energy and non-negative frequency in phonon spectra, respectively. Among the dynamically stable hetero-bilayers, binding energy in HBL 2 (AB1) is the lowest and interlayer distance ∼2.954 Å is the smallest. The HBLs are sensitive to the stacking arrangements, where HBL 2 demonstrates type-I direct bandgap and HBL 6 (AB6) is Type-II direct bandgap. The intrinsic HBLs show superior carrier mobility as their effective masses are lower from their constituent monolayers. Also, the intrinsic absorption coefficient of the HBLs increase as high as ∼10⁶ cm⁻¹, 10 times greater than conventional perovskite materials, which show outperforming optoelectronic conversion efficiency. Additionally, the HBLs are highly tunable in both bandgap and visible absorption peak by 3.5 (2) times in the HBL 6 (HBL 2). Electric fields also increase the photocatalytic water splitting performance with a net bandgap lowering and increasing the visible absorption peak by ∼1.5 times compared with intrinsic HBLs. These promising properties that we have found in the planar GaN/GeC vdW hetero-bilayer are highly suggestive for the impending use of this material in photocatalytic water splitting technology to produce H₂ fuel.

INDEX TERMS 2D GaN, hetero-bilayer, van der Walls (vdW) concept, first-principles density functional theory (DFT), optoelectronic property, photocatalytic water splitting, hydrogen (H₂) fuel.

I. INTRODUCTION
Among the total global energy consumptions, ∼90% of it comes from fossil fuels, which results in the high-emission of greenhouse gas, CO₂, responsible for global warming and climate change [1]. Also, carbon-based fossil fuels, which have a limited resource, are starting to scarce due to the incremental consumption of it [1]–[3]. Therefore, to overcome the negative effect of climate change, global warming, and mitigate the energy consumption demand, a renewable...
source of environment-friendly energy alternatives is highly required. The choice can be hydrogen (H$_2$), having high-energy conversion compared to fossil fuel, and becoming green fuel [4], as the burning of it produces water (H$_2$O). However, conventional H$_2$ production technologies, such as steam methane reforming (SMR) (∼ 900 ◦C of temperature, ∼ 15-3 MPa pressure required for H$_2$ production from natural gas) [5], coal gasification (∼ 5 MPa), and biomass pyrolysis [5], are high-cost and producing CO$_2$ by-product in some cases [5], [6]. That’s why water-splitting technology to produce hydrogen with comparatively low-cost and without CO$_2$ by-product can be a promising technology. Moreover, utilizing solar energy to produce hydrogen, facilitated by semiconductor-based photocatalysis, is an emergent topic in renewable solar energy conversion and green chemistry research. The process starts with the illumination of sunlight in semiconductors, resulting in the photogenerated charges (electron-hole pair), which then diffuse in the pure water and electrons (holes) contribute to hydrogen (oxygen) evolution reaction to produce H$_2$ (O$_2$) from water. To initiate photocatalytic water splitting in semiconductor, some conditions must be fulfilled [4]: (i) The conduction band edge (CBE) energy must be greater or equal to the reduction potential (∼−4.44 eV with respective to vacuum) or more negative than 0 eV versus NHE (normal hydrogen electrode) potential to produce hydrogen through reduction reaction (H$^+$/H$_2$), (ii) The valance band edge (VBE) energy must be smaller or at least equal to the oxidation potential (∼5.67 eV with respect to vacuum), or more positive than +1.23 eV vs. NHE energy to produce oxygen through oxidation reaction of water (O$_2$/H$_2$O), (iii) The semiconductor material must hold at least ∼1.23 eV of bandgap, (iv) It must have sufficient peak absorption in the near ultra-violet (NUV) and visible solar spectrum so that the high-intensity portion of the solar spectra can be utilized, and v) It must hold large surface to volume ratio so that the photocatalytic water splitting sites can be increased and redox reaction can be facilitated. Therefore, the core concern of the research in this field is to find out the materials that satisfy the above attributes for photocatalysis. From 1972, when the first photocatalytic water splitting in the TiO$_2$ bulk system was observed, a large number of materials, from bulk to nano, are investigated to enhance the photocatalysis performance, especially for water splitting technology to produce hydrogen [6]. However, acquiring novel materials that meet up all the conditions retain still a challenge.

With the novel exfoliation of graphene and its outperforming applications in various fields, many graphene-like nanomaterials and other nanostructures are investigated for photocatalysis so that the profound large surface to volume ratio in nanomaterial can be utilized. However, a couple of studies on TiO$_2$ material, the first photocatalyst, in its nanostructure (nanoparticle) form show better photocatalysis performance than the bulk system [7]–[9]. This evidence brings many two-dimensional (2D) materials involved in photocatalysis. Of them, graphene-like C$_3$N$_4$ (g-C$_3$N$_4$), a metal-free 2D photocatalyst, having ∼10 m$^2$/g surface area, and near UV bandgap ∼ 2.7 eV, show ∼ 3.2 µmol/h/g of H$_2$ yield for ∼ λ > 420 nm visible lights [10]. With Pt co-catalysts, it outperforms the yield of about ∼35 times more (∼106 µmol/h/g) [11]. Graphene with engineered bandgap and co-catalyst showed ∼1050 µmol/h/g yields [12]. Black phosphorene (BP), another intrinsic material like graphene, having ∼1.79 eV of bandgap, facilitates visible-light-driven photocatalysis [12]. Among 2D transition metal chalcogenides (TMDs) such as MoS$_2$, WS$_2$, MoSe$_2$, WSe$_2$ CdS, ZnS, SnS$_2$ are widely used for photocatalysis. Of them, MoS$_2$, MoSe$_2$, and WS$_2$ outperform as their H$_2$ yields are ∼ 26000, ∼ 62000, and ∼ 2570 µmol/h/g, respectively [13]. GaX (X = S, Se, Te) and InX (X = S, Se, Te) are also other kinds of 2D materials, having widely tunable bandgap (∼2.22-3.19 eV, ∼2.20-2.71 eV), are promisingly used in photocatalysis utilizing visible light [14]. All these nanostructures take advantage of the high-surface-area, resulting in enhanced photocatalytic active sites and enhanced carrier mobility. However, effective carrier separation to avoid the recombination and high-tunability in bandgap creates a limiting-phase of the nanostreams. To achieve these features, defect, elemental doping, co-doping, strains, external electric or magnetic fields, and van der Walls (vdW) heterostructure, etc. methods are being implemented widely. Among them, vdW hetero-bilayer, a comparatively lucrative concept, captures the core concentration in photocatalytic activity owing to its stacking patterns, interlayer spacings dependent on high-tunable bandgap, and effective spatial carrier separations [10], [11], [14]–[18]. In recent times, several studies are found on vdW-heterostructures for photocatalytic water splitting technology. Among them ZnO/MoS$_2$ [17], ZnO/WS$_2$ [16], blue phosphorene/g-GaN [15], blue phosphorene/ MoS$_2$ [14], graphene-g- C$_3$N$_4$ [11], BP/GaN [19], and GaN/GeC [20] are the few names. These materials show high-tailoring bandgap, high-absorption, stacking dependent tunability, and effective carrier separation, resulting in enhanced photocatalytic activities.

Although bulk GaN-research, especially in optoelectronics, has reached almost at the saturation level, the nanostructures of it are still in the infancy. The focus shifted on GaN-based nanomaterials is not more than a decade long. However, having wide electronic bandgap ∼4.18 eV-5.29 eV (experimental), with high-in-plane mechanical stiffness ∼108.37 N/m and a large Poisson’s ratio 0.410, high-thermal and chemical stabilities, strong-electric field supporting capabilities, the experimental realization of GaN nanostructures, and wide-spectrum promising application has made this structures a material of interest [21]–[30]. These features also motivated the material in its vdW form to be deeply studied for photocatalytic applications. Some prominent pieces of evidence are also seen in the literature for the application. They are compiled in TABLE 1. Among different methods of tailoring processes that are mentioned in the research community, the vdW realization of 2D planar GaN with 2D oxides and 2D TMDs become more popular. Some theoretical realizations
are MoS$_2$/GaN, phosphorene/GaN, GeC/GaN, BAs/GaN, and BP/GaN [31]–[37]. They all show stacking responsive bandgap altering nature, spatial separation of the carrier, and high-photocatalytic active sites, etc. Among them, GaN/GeC and BAs/GaN have enhanced UV-driven photocatalytic performance.

However, the utilization of the UV spectrum, which is only ~ 4% of total solar spectra, hinders the performance a lot from the optoelectronic carrier generation perspective [20], [34]. Moreover, the intrinsic 2D planar GaN (GaN-nanosheet) having UV ranged indirect bandgap and low-absorption in the visible spectrum, limit the application of the material in photocatalysis. To engineer the intrinsic material for photocatalyst and to introduce UV-visible shifting of optical absorption and indirect-direct bandgap transition for the GaN/GeC based vdW hetero-bilayer, intensive studies should be carried out. Also, to acquire the photocatalysis attributes of the materials, their strain, electric field, stacking dependent electronic and optical properties are needed to be studied. Therefore, in this work, we invoked to investigate the strain, electric field, stacking dependent electronic properties, photocatalytic overpotentials, effective masses, and optical absorption for the GaN/GeC vdW hetero-bilayer and showed that the fulfillment of the attributes is acquired. These studies also suggest that the materials in its hetero-bilayer form (vdW GaN/GeC) are highly promising for high-performance photocatalytic water splitting applications.

## II. COMPUTATIONAL METHODOLOGY

All the calculations in this study were done using Quantum Espresso [38] and Yambo in which density functional theory (DFT) based projected augmented wavefunction (PAW) method is hired. For the ground state electronic property, the Perdew-Burke-Ernzerhof (PBE) with generalized gradient approximation (GGA) exchange-correlation functional is utilized [39]. Norm conserving pseudopotentials (NCP) were implemented to describe electron-ion interactions. However, to predict accurate bandgap for semiconductors, conventional PBE functional is not sufficient. To overcome the bandgap problems, nonlocal hybrid functional, Heyd-Scusena-Ernzerhof (HSE 06) was applied in electronic property calculations for predicting the bandgap of proposed heterostructures. To further reduce the bandgap problem and achieve near experimental bandgap, we also used customized MGGA exchange-correlation functional with 2D PRHG-Regularized PBE [40]. The Grimme dispersion corrected DFT-D3 was applied so that vdW interaction between monolayers can be considered [41]. A 2 × 2 supercells of GaN and GeC monolayer were stacked on top of each other to model the vdW structures. A 20 Å vacuum along the perpendicular direction was allowed so that the inter-image layer interactions can be suppressed.

The maximum force, stress, and displacement tolerances were, 0.001 eV/Å, 0.05 GPa, and 5 × 10$^{-6}$ Å, individually, for structural relaxation and finding minimum energy configurations under Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm. The energy cut-off is 880 eV for kinetic energy. The Monkhorst-Pack K-points mesh of $12 \times 12 \times 1$, $16 \times 16 \times 1$, and $24 \times 24 \times 1$ are used for electronic band structure, projected density of states, and optical properties calculations, separately. The chemical stability predicting parameter, binding-energy of structures included in table 2, are equated by this equation,

$$E_b = E_{\text{heterobilayer}} - \sum_i E_i(\text{layer}_i)$$

where, $E_{\text{heterobilayer}}$ is the dispersion corrected entire energy of the hetero-bilayer system, and $\sum_i E_i(\text{layer}_i)$ is the sum of the energies of $i$ numbers of monolayers making the hetero-bilayer. Accordingly, charge density difference calculation equated the following equation,

$$\Delta \rho = \rho_{\text{heterobilayer}} - \sum_i \rho_i(\text{layer}_i)$$

here, $\rho_{\text{heterobilayer}}$ refers the hetero-bilayer system’s charge density and $\sum_i \rho_i(\text{layer}_i)$ is the accumulated charge density of the monolayers for making the vdW hetero-bilayers. Density functional perturbation theory (DFPT) was implemented on 2 × 2 supercells of all the structure for dynamical-stability-indicating phonon dispersion curves.

As an external perturbation for tuning the electronic properties, biaxial strains were applied, which can be equated as,

$$a_s = \pm e \times a_u + a_u$$

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**TABLE 1.** Photocatalytic water splitting technology facilitated by GaN-based vdW structures, 2D GaN, GaN nanotube in literature.

| Materials    | $E_g$(eV) | Utilized Spectrum | Remarks                        | Ref.  |
|--------------|-----------|-------------------|--------------------------------|------|
| ZnO/GaN      | 3.27-D    | UV                | Type-II, tunability absent     | [31], [32] |
| GaN/GeC      | 3.27 (GW), 1 | UV               | Type-II, tunability absent     | [20] |
| GaN/MoSe2    | 1.65-1.7 (HSE06), 1 | Visible           | Type-II, tunability present (slight) | [35] |
| GaN/WSe2     | 1.7-1.8 (HSE06), D | Visible           | Type-II, tunability present (slight) | [35] |
| GaN/BAs      | 1.7 (HSE06), D | Visible           | Type-II, tunability absent     | [34] |
| MoSe2/GaN    | 1.5 (HSE06), D | NIR, Visible      | Type-II, tunability absent     | [37] |
| BP/GaN       | 1.6 (HSE06), D, 1 | Visible           | Type-II, tunability present     | [19] |

D = direct bandgap, I = indirect bandgap, Vis = visible, NIR = near infra-red, UV= ultra-violet.
where, \(a_s\) and \(a_u\) denotes lattice constants of strained and unstrained structural models, correspondingly. The \(e\) denotes the strain magnitude. The +ve and -ve signs refer to the tensile and compressive strains, respectively.

To model the electromagnetic illumination’s response in the semiconductor, we followed the complex dielectric function equated as, \(\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)\). A direct correlation can be found between the cross-band energies of the electronic dispersion and the imaginary part of the dielectric function. This co-relation can be visualized from the filled and unfilled states equation,

\[
e_2 = \frac{2e^2\pi}{\Omega\varepsilon_0} \sum_{k,v,c} \left| \langle \psi_k^v | \hat{\mu} \times \hat{r} | \psi_k^c \rangle \right|^2 \delta(E_k^c - E_k^v - E)
\]

where \(e\) infers the charged electron, \(\hat{\mu}\) represents polarization vector of occurrence field, \(\Omega\) refers to the polarization density, \(\hat{r}\) denotes the spatial position, \(\psi_k^v\) and \(\psi_k^c\) are the conduction band (CB) and valence band (VB) wave-function at wave vector \(k\), singly. \(E_k^c\), \(E_k^v\), and \(E\) embody the energy of CB, valance band energy, and Fermi energy, one-to-one.

**III. RESULTS AND DISCUSSION**

**A. STRUCTURAL PROPERTIES**

The structural insights of our proposed materials, starting from GeC/GaN hetero-bilayers, are studied systematically. The optimized structures are shown in Fig 1. All the consisting monolayers are found planar honeycomb structure with zero buckling. We have calculated the geometry-relaxed parameters i.e., lattice constant, \(a\) and bond lengths. It is found that \(a = 3.248\) Å and bond-length 1.875 Å for planar GaN monolayer. For GeC monolayer, the lattice constant \(a\) is 3.268 Å with a bond length of 1.887 Å [20]. These data are in good correspondent with former studies [26], [42], [43]. The stacking is made in such a way that the 2\(\times\)2 GeC (\(a = b = 6.536\) Å) monolayer is the bottom layer, and the 2\(\times\)2 planar GaN (\(a = b = 6.496\) Å) is vertically placed on the layer in six different stacking patterns. Having the same type of crystal structures and close-matched lattice constants, lattice mismatch becomes only \(\sim 0.61\)%, remarkably small compared to other vdW hetero-bilayers. The six stacking patterns that we have adopted are: In HBL 1 (AA), Gallium (Ga) and Nitrogen (N) atoms are straight on the upper side of Germanium (Ge) and Carbon (C) atoms, individually; in HBL 2 (AB1), N(Ga) atoms are right on the upper side of Ge (C) atoms; In HBL 3, Ga atoms are straight on the upper side of Ge atoms and N atoms are in the middle of hexagons; In HBL 4, G atoms are unswervingly on top of C and N atoms are in the middle of hexagons; In HBL 5, Ga atoms are in hollow while N atoms are right on top of Ge atoms; lastly, in HBL 6 (AB6), N atoms are straight on top of C atoms and Ga atoms are placed in the middle of hexagons. Room temperature thermodynamic stability can be predicted by density functional perturbation theory (DFPT) based phonon spectra calculations. The HBLs 1, 3, 4, and 5 are found dynamically unstable due to imaginary branches in the phonon spectra (see APPENDIX Figs. A1(a - h)); this proceeds with excluding the hetero-bilayer from the next studies.

The geometry-relaxed and dynamically stable structures have lattice constants \(\sim 3.261\) Å, and \(\sim 3.252\) Å for HBL 2, and HBL 6, correspondingly. The data are within the lattice constants of planar GaN and GeC monolayer, as expected from theory. Among the HBLs, HBL 2 (AB1) has the smallest interlayer spacing \(\sim 2.954\) Å, while HBL 6 has an interlayer distance of \(\sim 3.115\) Å.

For exploring the energetically favorable stable model, the inter-layer binding energy is evaluated with inter-monolayer spacing as a variable utilizing the formula,

\[
E_b = E_{\text{GaN/GeC heterobilayer}} - E_{\text{GaN}} - E_{\text{GeC}}
\]
where, $E_{\text{GaN/GeC heterobilayer}}$ denotes dispersion corrected total enthalpy of the hetero-bilayer, $E_{\text{GaN}}$ refers the energy of planar GaN monolayer and $E_{\text{GeC}}$ indicates the total energy of GeC monolayer. The interlayer-dependent binding energy plots for HBL 2, and HBL 6 are demonstrated in Fig.2. The interlayer binding energy, corresponding interlayer spacings, geometry-relaxed lattice constants, and bond lengths are abridged in TABLE 2. The binding energy is significant that it can suggest the most energetically favorable hetero-bilayer. From the binding energy of hetero-bilayers, HBL 2 appears to be the greatest energetically advantageous, indicating its tentative practicability. In the interim, HBL 6 has the uppermost binding energy unswerving with the highest interlayer spacing.

![FIGURE 2. Binding energy vs. interlayer distances.](image)

### B. ELECTRONIC PROPERTIES OF HETERO-BILAYER SYSTEM

First, the comparative electronic dispersion curves via PBE, HSE 06 non-local hybrid functional, and MGGA (with 2D PRHG corrected exchange and PBE regularized GGA correlation) of GaN and GeC monolayer are compared to validate our user-defined exchange-correlation functional for ongoing implementations. The bandgap value predicted by PBE, HSE 06, GW, experimental, and MGGA functional of GeC and GaN monolayers are demonstrated in Figs. 3 (a), (b), and (c). The bandgaps clout a close match with the previous theoretical and experimental studies [20], [28], [31], [42]–[44]. Interestingly, our customized functional show acceptable accuracy compared with high-accurate GW approximation (∼3% deviation from GW in 2D GeC and ∼5% deviation from GW in 2D GaN) and experimental (our proposed MGGA underestimates 2D GaN bandgap ∼0.82 eV while GW approximation underestimates the bandgap ∼1.04 eV). These comparisons suggest that the customized MGGA we have adopted is in a close match with the experimental bandgap with an approximately 95% reduction of the computational cost compared with other non-local hybrid functional (e.g., HSE06 requires 48 CPU hours while MGGA requires only 2 CPU hours for the same type of calculations). The MGGA band-structures of hetero-bilayer HBL 2 and HBL 6 are exhibited in Figs. 3 (e) and (d), correspondingly. It is found that the bandgap values (types) are highly receptive to the stacking pattern of the hetero-bilayers. As presented in Fig. 3(c), hetero-bilayer model 2 has direct bandgap electronic property (type-I) while another dynamically stable hetero-bilayer model is found direct bandgap (type-II), highly necessitated for photocatalytic implementations.

The bandgaps of all two hetero-bilayers are compared with different functionals in TABLE 2. The comparative band structures calculated by HSE-06 functional are also shown in the black line in the Figs. 3(c) and (d), respectively. For suggesting photocatalytic water splitting activities, band-edge position calculation is highly required. To explore the band-edges, MGGA bandgaps are taken into consideration involving the equation $E_{\text{CB}} = X - E_e - (E_{\text{MGGA}}/2)$ for conduction band edge and $E_{\text{VB}} = X - E_e + (E_{\text{MGGA}}/2)$ for valance band edge calculation. The X refers to the geometric mean of the Muliken electronegativities of the encompassing atoms of the hetero-bilayers, $E_e$ epitomizes the free electron energy compared to the hydrogen scale (4.5 eV). In our study, the Muliken electronegativities for GaN, and GeC monolayers are 4.83 eV and 5.34 eV, correspondingly. Fig 3(d) shows the comparative band edge locations of GeC, GaN, and our projected hetero-bilayers. It illustrates that the valence band maxima are subsidized by GaN monolayer while conduction band minima are contributed by GeC monolayer, resulting in type-II band alignment in HBL 6. The (2H$^+/H_2$) reduction potential at −4.46 eV energy level and (H$^/_2/O/O_2$) oxidation potential at −5.67 eV energy level are shown to reconnoiter the likely photo-catalytic over-potential of the hetero-bilayers.

![FIGURE 3. The electronic dispersion curves for (a) GaN monolayer (2D GaN), (b) GeC monolayer (2D GeC), (c) bandgap values by different methods, band structure for (d) HBL 2 and (e) HBL 6. Fig (f) shows relative band alignment for GeC, GaN, HBL2, and HBL6 for photocatalytic water splitting.](image)
HBLs 2 and 6 have adequate dynamic over-potential to inductee the photocatalysis as the conduction band edge (valance band edge) has higher (lower) energy than oxidation (reduction) potential. The valance band offset (VBO) and conduction band offset (CBO) are 0.067 and 0.967 eV, individually, signifying operative carrier parting, which is exceedingly required for photocatalysis.

To additional inspect the atomic orbital influence in the band ends, the total and partial density of states are revealed in Figs. 4 (a) and (b). In HBL 2, the conduction band minima (CBM) is mainly subsidized by Ge atom, to be specific SP$^2$ hybridized p-orbital of GeC monolayer and the valance band maxima (VBM) is parted by the C atom of GeC monolayer predominantly, again from SP$^2$ hybridized p-orbital, which consequences type I straddling band position in HBL 2. On the contrary, in HBL 6, the VBM is mainly underwritten by p-orbital of N atoms of GaN monolayer, while CBM is mostly subsidized from p-orbital of Ge atoms of GeC monolayer, suggesting type II staggered band orientation.

Work function calculation was introduced to find out the direction of electron allocation in GaN/GeC HBLs. The work function defined as $W = E_{\text{vacuum}} - E_{\text{Fermi}}$, i.e., the substraction between the energy for going electron to vacuum and the energy of the Fermi level. The work functions of the GeC and GaN monolayers are 4.75 eV and 5.18 eV, individually. Having the truncated work function value of GeC comparable to GaN monolayer, it can correspondingly be surmised that the electrons unswerving from GeC to GaN monolayer when hetero-bilayers to be designed until equipoise is gotten between the Fermi levels. The work functions of HBL 2 and HBL 6 are 5.063 eV and 5.092eV, respectively. The values deduce that the work-function is also reactive to the assembling patterns of the hetero-bilayers.

Besides, the charge (electron) density change of the HBLs is confirmed in Figs. 5 (a-b) following the reckoning, $\Delta \rho = \rho_{\text{HBLs}} - \rho_{\text{MLGeC}} - P_{\text{MLGaN}}$, where, $\rho_{\text{HBLs}}$ is the charge density of the hetero-bilayers, $\rho_{\text{MLGeC}}$ is the charge density of GeC monolayer and $P_{\text{MLGaN}}$ is the charge density of the GaN monolayer. The red and yellow region signifies the charge accumulation and depletion, correspondingly. In HBL 2 (Fig 5. (a)), Ge (C) predominantly depletes (accumulates) the charges, in which C atom mushrooms the charge depleted by Ga atoms and Ge depletes the charges gathered by N atoms. In the HBL 6 (Fig 5 (b)) system, alternatively, charges amass in the interfacial section washed-out by Ge atoms primarily. These features are similarly invertebrate by charge density deviation at the edge of HBLs revealed in Figs 5 (c) and (d). Additionally, a sturdier interfacial connection of hetero-bilayers can be advised by the degree of interfacial charge circulation. Our calculation suggests that the uppermost charge redeployment transpires in HBL 2, confirmative to its small-interlayer spacing and sturdy binding energy.

Succeeding the charge density difference, the electrostatic potentials of the HBLs via the Poisson equivalence. 2D GeC has a higher potential than 2D GaN, which is reliable with the charge transmission. A noteworthy potential drop of $\sim3.75$ eV is attained in our scheming. This high-potential difference denotes a stout electrostatic electric field, which can proficiently discrete the charge carriers, portentous of little-probability of recombination, exceedingly operative for photocatalysis. We have equally computed the electron effective mass of our planned monolayer and hetero-bilayers to have additional intuition into carrier dynamics, which tabulated in TABLE 3. Our calculations propose that the electron-effective masses are also reliant on stacking decorations. Surprisingly, the electron effective mass
in the hetero-bilayer systems is lower than the comprising monolayers, which refers to the high-carrier mobility in the hetero-bilayer systems. This low-electron effective mass (high-mobility) suggests the low-recombination time of carrier and efficient carrier separation, highly required for photocatalytic water splitting and photovoltaic applications.

### C. STRAIN DEPENDENT ELECTRONIC PROPERTIES FOR HBLS

Smearing strain is one of the weighty ways to control the electronic characterization of heterostructures as it is self-induced owing to lattice discrepancy, imperfection, and impurities at the time of fabrication. Thus, biaxial strains are deployed to show how it marks the inherent electronic properties of GaN/GeC HBLs. The tempered bandgaps with compressive (negative) and tensile (positive) strain are publicized in Figs. 6 (a-d). The electronic dispersions show incredibly subtle to the biaxial strain in their bandgaps and direct to indirect changeovers. For HBL 2, the unstrained band structure is a direct gap at K to K point. When compressive strain is applied, it becomes an indirect bandgap at K to M point precisely for 2%, 4%, and 6% of compressive strain shown in Fig. 6 (a). When tensile strain is applied, it again relics indirect for 2%, 4%, and 6% as confirmed in Fig. 6 (b). It seems that both compressive and tensile strain in HBL 2 changes the bandgap from direct to indirect, which is undesired. However, the bandgap values are lowered almost by two times for compressive to tensile strains in both GGA-PBE and MGGA exchange-correlation calculations, as compiled in Figs 6 (e) and (f). In the case of HBL 6, the unstrained HBL is a direct bandgap, and it sustains this feature at all compressive strains shown in Fig. 6 (c). However, for all tensile strains, it becomes an indirect bandgap, as shown in Fig. 6 (d). Again, the bandgap values are lowered by the factor of two for compressive to tensile strains. The low-bandgap facilitates the photocatalytic activities because of UV to the visible transition of absorption. Thus, biaxial strain-induced electronic property modulation is an essential feature for the material systems, especially in hetero-bilayer systems.

However, the band edge position must be so that the CBE is higher than the reduction potential, turning water into hydrogen and VBE is lower than the oxidation potential, turning water into oxygen. Therefore, we have calculated the relative band edge position for strain-induced HBL 2 and HBL 6, as depicted in Figs 7 (a), (b). The lowest bandgaps obtained upon applying 6% tensile strain are \( \sim 1.83 \text{ eV} \) for HBL 2 and HBL 6. They both have sufficient kinetic overpotential with the values \( \sim 0.27 \text{ eV} (\sim 0.19 \text{ eV}) \) in CBE and \( \sim 0.32 \text{ eV} (\sim 0.26 \text{ eV}) \) in VBE for HBL 2 (HBL 6). Conversely, the highest kinetic overpotentials are obtained \( \sim 1.43 \text{ eV} (\sim 1.29 \text{ eV}) \) in CBE and \( \sim 1.48 \text{ eV} (\sim 1.35 \text{ eV}) \) in VBE for HBL 2 (HBL 6). These values suggest that the HBL systems can be a potential entrant for photocatalytic water splitting with high-tunability in kinetic overpotential.

### D. ELECTRIC FIELD DEPENDENT ELECTRONIC PROPERTIES FOR HBLS

Cross-plane electric filed is another tool for bandgap engineering. Graphene shows bandgap under a perpendicular
electric field. Conversely, hetero-bilayer materials such as GeC/GaS, GeC/SiC show diminishing bandgap with $\sim \pm 0.5$ V/Å. We have applied the perpendicular electric field in the positive (bottom layer to top layer direction) and in the negative direction (top layer to bottom layer direction). It turns out that $\sim \pm 2.5$ V/Å electric field vanishes the bandgap in our GaN/GeC HBLs. However, photovoltaic and photocatalytic applications require a bandgap above zero. Therefore, the external electric field range chosen is from $-1.0$ V/Å to $+1.0$ V/Å. Fig 8 (a) represents the electric-field dependent bandgap values. The schematic diagrams of applied electric field directions for HBL 2 and HBL 6 are revealed in Figs 8 (b) and (c), individually. With the increase in electric field up to $+1$ V/Å in the positive direction, the bandgap value is linearly decreasing, and the direct-indirect bandgap splitting is also increasing as demonstrated in Fig 8 (a). In (APPENDIX Fig. A2 (a)), the band-structure plots with positive electric fields also confirm the phenomena. It shows that with increasing electric fields in the positive direction, the valance bands near K points are shifting toward the Fermi energy level while the conduction bands, specifically bands at Gamma point, are shifting toward the Fermi level, originating the lowering of the bandgap. Meanwhile, the band at K point in the CB also shifts toward a high-energy level, resulting in a rise in the K to K direct band-gap. However, when the field direct altered, i.e., in the negative direction, the CB is almost constant except the bands at M point shifting toward Fermi level while the valance band changes randomly with a shifting of a band near K point toward Fermi level. Thus, the bandgap upon applying a negative electric field is lowered with a slight splitting between direct-indirect bandgap. As a whole, the band-shifting results in the band-splitting more appearing due to a positive field than band splitting due to the negative electric field in HBL 2.

In the case of HBL 6 (as portrayed in Figs 8 (a), (c) and APPENDIX Fig. A2 (b)), for the positive electric field, again, the bandgap is lowered monotonically, and the negative electric field also follows the trends of bandgap lowering. The positive electric field keeps VB almost constant with a net increase in energy level at K point while bands at G point are lowering, resulting in the bandgap lowering with direct-indirect bandgap transition (at $+0.2$ V/Å). Oppositely, due to the negative electric field, the CB becomes almost constant with a net shifting of bands at K point toward Fermi level while the VB shifts toward Fermi level at K point, resulting in direct bandgap with a monotonic decrease in bandgap values. This nature shows low-band-splitting in HBL 6 compared with HBL 2.

To explore the bandgap nature (Type-I or Type-II), necessary for photocatalytic and photovoltaic applications due to effective carrier separation, we calculated the atom projected band-structures (shown in APPENDIX Fig A2 (a) and (b)) and atom projected DOS (given away in Figs 9 (a) and 10 (a) for HBL 2 and HBL 6, correspondingly). In HBL 2 when $+0.2$ V/Å is applied, the atom projected and PDOS show that the VBM is mainly provided by C atoms, and CBM is mostly provided by Ge atoms, i.e., CBM and VBM are primarily contributed by GeC monolayer, indicating Type-I band alignment. Remarkably, in all other positive electric fields from $+0.4$ V/Å to $+1.0$ V/Å, the VBM is principally donated by C atoms, while CBM is dominated by Ga atoms, referring
to Type-II band alignment. Interestingly, for negative electric field ranges from $-0.2$ V/Å to $-1.0$ V/Å, the VBM is mainly contributed by N atoms of GaN monolayer while CBM is dominated by Ge atoms of GeC monolayer, which depicts Type-II band alignment as well. HBL 6 also follows a similar fashion in-band alignment, i.e., for $+0.2$ V/Å it becomes Type-I (VBM from C and CBM from Ge) and in all other electric fields, it becomes Type-II (for the positive field, VBM from C and CBM from Ga while for negative fields VBM from N and CBM from Ge).

We also calculated the relative band edge positions for applied electric fields for HBL 2 and HBL 6 so that the photocatalytic water splitting can be explored. It appears that in HBL 2, all have sufficient kinetic overpotential for photocatalysis except for $+1.0$ V/Å as pictured in Fig 9 (b). On the contrary, for the $-0.6$ V/Å to $+0.8$ V/Å range, the HBL 6 has sufficient kinetic overpotential to initiate photocatalysis. For other applied electric fields, it doesn’t fulfill photocatalysis energy requirements, as demonstrated in Fig 10 (b). Conclusively, the highest kinetic overpotential obtained at $-0.2$ V/Å for HBL 2 and $+0.2$ V/Å for HBL 6.

E. TUNABILITY IN OPTICAL PROPERTIES

1) INTRINSIC OPTICAL PROPERTIES

Ensuing the electronic properties and their cadences because of biaxial strain and electric fields, the optical properties specifically, dielectric functions and absorption co-efficient with varying photon energy, are considered by MGGA (2DHG-RPBE) exchange-correlation functional. The complex dielectric function ($\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$) reveals the response of the semiconductive medium owing to light reliant on angular frequency ($\omega$). Dielectric physics portrays that the real part, $\varepsilon_1(\omega)$ (imaginary part, $\varepsilon_2(\omega)$) is closely related to the dispersion effect (absorption loss). The compatible absorption coefficient with variable energy can also be calculated using the real and imaginary portions of the dielectric equation,

$$\alpha_\omega = \sqrt{2}[\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega) - \varepsilon_1(\omega)]^{1/2}$$

where $\alpha_\omega$ epitomizes the absorption co-efficient and $\omega$ denotes photon frequency. The real, imaginary share of complex dielectric function and absorption coefficient with the photon energy range of 0 to 20 eV are confirmed in Figs. 11 (a-c). Amazingly, the real part $\varepsilon_1$ for HBL 2 and HBL 6 is negative within the $\sim 7.2$ eV to 10.0 eV range, telling the metallic flavor of the hetero-bilayer. This attribute can divulge the probable implementation of the material for nano-coating in the ultra-violet (UV) region. Besides, they show positive $\varepsilon_1$ in the visible and near UV region, denoting their high-refractive semi-conductivity. Besides, in the imaginary dielectric part, the pedigrees and crests are also considered, matching with other works. The roots of the absorption peaks in the imaginary dielectric portion, as portrayed in Fig. 11 (b), are at $3.4$ eV, and $3.42$ eV for HBL 2, and HBL 6, respectively, affable with the bandgaps under MGGA DFT. Our calculation points out that all the HBLs have superior absorption compared with it’s founding GaN and GeC monolayer in the solar spectra. The maximum absorption attained is $\sim 1 \times 10^6$ cm$^{-1}$ for HBL 6 at $\sim 6.6$ eV, analogous with perovskite, and competent for optoelectronic devices [45]. The cumulative amount of electron-hole pair cohorts are connected to the growth of absorption points, it recommends the high-latency for photocatalysis of the HBLs. Furthermore, the greater amounts of peaks infer that more carrier conversions in HBL 2 and HBL 6, which is also reliable with our electron transfer study. Moreover, in the near-visible range ($\sim 3.4$ eV) the absorption coefficient is as significant as $\sim 4 \times 10^5$ cm$^{-1}$.

2) STRAIN AND ELECTRIC FIELD INDUCED OPTICAL ABSORPTION

Though it is comparable to perovskite material, high-absorption in UV suggests that the HBLs at intrinsic conditions are suitable for UV assisted photocatalysis.
The high-bandgap-originated UV absorption can be shifted towards visible through applying strain and electric fields so that the full solar spectra can be utilized. Therefore, we have calculated the strain and electric field modulated absorption co-efficient with varying photon wavelengths for HBL 2 and HBL 6 as depicted in Figs. 12 and 13. It shows in Figs. 12 (a) and (b) that in HBL 2 the unstrained absorption peaks ~ $10^5$ cm$^{-1}$ in the visible region (~ 380 nm). However, positive strains +2%, +4%, +6% are shifting the peaks towards UV, which consistent with the bandgap values, as mentioned in the electronic properties section. Interestingly, at compressive strains, specifically, at −4% and −6%, the absorption peaks in the visible region becomes almost three times that of the intrinsic peak, suggesting high-photocatalytic activity with enhanced carrier generations. In the case of HBL 6, the compressive strains also enhance the absorption peak in the visible region, and it becomes as high as ~ $3.5 \times 10^5$ cm$^{-1}$, suggesting high-efficiency in photocatalysis for HBL 6 compared with HBL 2. The electric field’s application also shows high-modulation in absorption peaks in the visible region.

However, the electric field that fulfills the goal i.e., high-absorption in the visible with sufficient kinetic overpotential for photocatalysis − 1.0 V/Å to −0.6 V/Å with ~ $10^5$ cm$^{-1}$ absorption coefficient for HBL 2 as referred in Fig 13 (a), (b). However, in HBL 6 within the −0.6 V/Å to +0.6 V/Å range, it shows a high-absorption coefficient with sufficient kinetic overpotential. Hence, with a wide range of electric field responsive absorption modulation, the HBL 6 is more...
promising than the HBL 2. It is worth mention that at the negative electric field, the HBL 6 has a direct type-II bandgap, which is highly required for photocatalytic water splitting and photovoltaic applications.

**IV. CONCLUSION**

Photocatalytic water splitting in GaN/GeC vdW heterobilayers are investigated under the first-principles DFT framework. The dynamical stabilities of the HBL systems are assured by the phonon spectra. Amongst the two dynamically stable HBLs, HBL 2 shows the lowest interlayer distance with the lowest binding energy, expressing its experimental feasibility of formation and chemical stability. The intrinsic HBLs show a wide electronic direct bandgap of $\sim 3.47$ eV, and $\sim 3.38$ eV for HBL 2 and HBL 6, respectively. For all biaxial strains (both compressive and tensile) the band edges have sufficient kinetic overpotential for photocatalytic water splitting with a net monotonic lowering of the bandgap for tensile strains. Because of the application of biaxial strain, direct-indirect bandgap transition occurs and direct-indirect gap splitting is more visible in HBL 2 than in HBL 6. For cross-plane external electric fields, in both HBLs the bandgap is lowered almost two times. Moreover, in HBL 2, the band edges have sufficient kinetic overpotential within the $\sim -1.0$ V/Å to $+0.8$ V/Å electric field range. For HBL 6, the permissible range reduces to $\sim -0.6$ V/Å to $+0.8$ V/Å. The co-dopant structures have also shown an indirect-direct bandgap transition with sufficient kinetic overpotential. The electron effective mass in HBLs is lower than the comprising monolayer, suggesting high-carrier mobility in HBLs. The intrinsic optical properties show that the high-absorption coefficient of $1 \times 10^6$ cm$^{-1}$ remains in the UV range for the HBLs. The biaxial strains and electric fields can successfully tune the optical peak absorption with a net $\sim 10^5$ cm$^{-1}$ in the visible spectrum. The strains in HBL 6 (HBL 2) increases the absorption peaks in the visible by almost $\sim 3.5$ (2) times greater than the intrinsic HBLs. Electric fields, on the other hand, increases the peak by $\sim 1.5$ times compared with intrinsic HBLs in the visible solar spectra for a permissible range of photocatalysis.

**APPENDIX**

To clarify the dynamical stability, phonon dispersion has been calculated for different structures as shown in Figs. A1 (a-h). Electric field dependent atom projected electronic band-structures for (a) HBL 2, and (b) HBL 6 have also represented in Figs. A2 (a-h).

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MD. SAKIB HASAN KHAN received the B.Sc. and M.Sc. degrees in electrical and electronic engineering from the Khulna University of Engineering & Technology (KUET) in 2018 and 2020, respectively. He has been serving as a Lecturer with KUET since 2018. He has authored or coauthored research articles in national and international conferences and journals. His core research interest includes optical properties of 2-D materials and their applications in hydrogen fuel production.

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MD. RAFIQUIL ISLAM (Member, IEEE) received the B.Sc. degree in electrical and electronic engineering from the Bangladesh University of Engineering and Technology, Dhaka, Bangladesh, in 1998, the M.Sc. degree in electrical and electronic engineering from the Khulna University of Engineering & Technology (KUET), Khulna, Bangladesh, in 2006, and the Ph.D. degree in semiconductor device growth, characterization, and fabrication from the University of Fukui, Japan, in 2010. He is currently a Professor with KUET. He has authored or coauthored more than 50 research articles in national and international conferences and journals. His research interests include thin films solar cells, growth characterization and fabrications, advanced semiconductor materials properties, and compound semiconductor-based devices. He received the MONBUKAGAKUSHO scholarship from Japan (MEXT, 2007–2010). His two articles received the Best Paper Award at international conferences.

MD. TANVIR HASAN (Member, IEEE) received the B.Sc. and M.Sc. degrees in electrical and electronic engineering from the Khulna University of Engineering & Technology, Bangladesh, in 2006 and 2007, respectively, and the Ph.D. degree in electrical and electronic engineering from the Graduate School of Engineering, University of Fukui, Japan, in 2013. He is currently an Associate Professor with the Department of Electrical and Electronic Engineering, Jashore University of Science and Technology, Bangladesh. He has authored or co-authored more than 50 research articles in conferences and journals. He has been a member of the IEEE Electron Devices Society since 2008. His research interests focus on growth, design, fabrication, characterization, simulation, and modeling of III–V-based semiconductor devices (electronic and optoelectronic). He served as a Secretary and an Executive Committee Member for the IEEE Young Professional of Bangladesh Section (BDS) and a Professional Activity Coordinator for the IEEE BDS in 2016 and 2017, respectively. He received the MONBUKAGAKUSHO scholarship from Japan (MEXT, 2010–2013). He received the IEEE Student Paper Award (Honorary Mention) from the IEEE Electron Devices Society, Bangladesh Chapter, in 2007. He serves as a Reviewer for the IEEE TRANSACTIONS ON ELECTRON DEVICES, the Journal of Applied Physics, and Applied Physics Letters.

MUHAMMAD SHAFFATUL ISLAM received the B.Sc. degree in electrical and electronic engineering from American International University-Bangladesh (AIUB), Dhaka, Bangladesh, in 2010; the M.Sc. degree in electrical and electronic engineering from the Khulna University of Engineering & Technology (KUET), Khulna, Bangladesh, in 2015. He is currently a Lecturer with the Department of Electrical and Electronic Engineering, World University of Bangladesh (WUB), Dhaka. His current research interests include III–V-based single- and double-gate MOSFET and the crystal orientation dependent characteristics of devices.

IBRAHIM M. MEHEDI received the B.Sc. degree (Hons.) in electrical and electronic engineering from the Rajshahi University of Engineering and Technology, Bangladesh, in 2000, and the M.Sc. degree in aerospace engineering from Universiti Putra Malaysia, Malaysia, in 2005, and the Ph.D. degree in electrical engineering and information systems from The University of Tokyo, Tokyo, Japan, in 2011. He was with the Coca-Cola Bottling Plant for two years. He was appointed as a Lecturer with the King Fahd University of Petroleum and Minerals in 2006. He was a Research Assistant and a Post-Doctoral Fellow with the Japan Aerospace Exploration Agency, Japan, from 2008 to 2012. He joined the Department of Electrical and Computer Engineering, King Abdulaziz University (KAU), in 2012, where he is currently an Associate Professor. He is a Senior Scientist with the Center of Excellence in Intelligent Engineering Systems, KAU. He has been involved in several research and development projects. He was the Principal Investigator in large research and development projects funded by KACST, MOE, and KAU. He has authored or coauthored several journals and conference articles and supervised and cosupervised several M.Sc. and Ph.D. students. His field of interests and specializations covers a broad spectrum from theoretical to practical aspects of engineering, including intelligent systems, control, electronic devices, sensors, energy, and artificial intelligence.

MD. TANVIR HASAN (Member, IEEE) received the B.Sc. and M.Sc. degrees in electrical and electronic engineering from the Bangladesh University of Engineering & Technology, Bangladesh, in 2006 and 2007, respectively, and the Ph.D. degree in electrical and electronic engineering from the Graduate School of Engineering, University of Fukui, Japan, in 2013. He is currently an Associate Professor with the Department of Electrical and Electronic Engineering, Jashore University of Science and Technology, Bangladesh. He has authored or co-authored more than 50 research articles in conferences and journals. He has been a member of the IEEE Electron Devices Society since 2008. His research interests focus on growth, design, fabrication, characterization, simulation, and modeling of III–V-based semiconductor devices (electronic and optoelectronic). He served as a Secretary and an Executive Committee Member for the IEEE Young Professional of Bangladesh Section (BDS) and a Professional Activity Coordinator for the IEEE BDS in 2016 and 2017, respectively. He received the MONBUKAGAKUSHO scholarship from Japan (MEXT, 2010–2013). He received the IEEE Student Paper Award (Honorary Mention) from the IEEE Electron Devices Society, Bangladesh Chapter, in 2007. He serves as a Reviewer for the IEEE TRANSACTIONS ON ELECTRON DEVICES, the Journal of Applied Physics, and Applied Physics Letters.