A van der Waals Heterostructure Based on Graphene-like Gallium Nitride and Boron Selenide: A High-Efficiency Photocatalyst for Water Splitting

Kai Ren,† Yi Luo,* Sake Wang,* Jyh-Pin Chou,† Jin Yu,‡ Wencheng Tang,*† and Minglei Sun*†‡

†School of Mechanical Engineering and ‡School of Materials Science and Engineering, Southeast University, Nanjing, Jiangsu 211189, China
§College of Science, Jinling Institute of Technology, Nanjing, Jiangsu 211169, China
∥Department of Mechanical Engineering, City University of Hong Kong, Kowloon, Hong Kong 999077, China

ABSTRACT: Hydrogen generation by photocatalytic water splitting has attained more and more research interests in the recent years since the solar energy can be directly transferred and stored as hydrogen. However, the search for a high-efficiency photocatalyst for water splitting is a really challenge. In this paper, we designed a novel 2D material-based van der Waals heterostructure (vdWH) composed by g-GaN and BSe, which is thermally stable at room temperature. The g-GaN/BSe vdWH has suitable band-edge positions for the oxidation and reduction reactions of water splitting at pH 0 and 7. The carrier mobility of this heterostructure is high, indicating the effective occurrence of reactions for water splitting. The g-GaN/BSe vdWH also possesses a type-II band alignment, which can promote the separation of the photogenerated electron–hole pairs constantly. Moreover, a large built-in electric field can be established at the interface, which will further prevent the recombination of photogenerated charges. In addition, the g-GaN/BSe vdWH also exhibits outstanding sunlight-absorption ability, and the biaxial strain can further enhance this ability. Thus, we conclude that the g-GaN/BSe vdWH can act as a high-efficiency photocatalyst for water splitting.

INTRODUCTION

The adoption of clean energy has become more and more important as the sources of fossil fuels around the world are depleted. Hydrogen (H₂) is a well-known green energy source because the product of hydrogen burning is water (H₂O). There are many strategies for hydrogen production, such as electrolysis of water,¹⁻⁶ thermochemical splitting of water,⁷⁻⁹ catalytic reforming,⁸⁻¹⁰ and photocatalytic water splitting,¹¹⁻¹³ etc., but it is quite challenging to find a photocatalyst with high efficiency in photocatalysis for water splitting. Ever since Fujishima and Honda have promoted in 1972 that an electrode based on TiO₂ can decompose water into H₂ and O₂ via near-ultraviolet light at room temperature,¹³ there have been many investigations on the use of semiconductors as photocatalysts for water splitting.¹⁴⁻¹⁶ The essential criteria for a semiconductor to serve as a photocatalyst in water splitting are suitable band-edge positions for the redox potentials of water splitting; the energy of conduction band minimum (CBM) is more positive than −4.44 eV, which is the reduction potential (H⁺/H₂) of water at pH 0; the energy of valence band maximum (VBM) is more negative than −5.67 eV for the oxidation potential (O₂/H₂O) of water at pH 0;¹⁷ then, the bandgap now is larger than 1.23 eV. In addition, the semiconductor must have the ability to absorb sunlight, especially for visible light, because the visible spectrum occupies more than 40% of the solar spectrum.¹⁸

Using two-dimensional (2D) materials as photocatalysts to decompose water into H₂ and O₂ have dominated research efforts because of their novel electronic, optical, magnetic properties when compared with those of bulk materials.¹⁹⁻²¹ First, a high specific surface area, for example, the specific surface area of the graphene sheet is 2600 m²·g⁻¹, which guarantees the reaction on their surface, will occur in an effective manner.²² Second, atomically thin structures reduce the time it takes for photogenerated charges to move to the surface, which can prolong the lifetime of photogenerated electron–hole pairs.²³ Therefore, 2D materials are a better candidate for photocatalysts in water splitting than the bulk materials. Indeed, lots of investigations have reported that the 2D materials, such as graphene,¹⁰ monolayer group III monochalcogenide,¹¹ phosphorene,²⁴⁻²⁶ and transition metal dichalcogenides (TMDs),²⁷⁻²⁹ may have the ability to split water under the illumination of visible light. Moreover, the formation of heterostructures may generate properties that are...
more fascinating than those of the original 2D materials.\textsuperscript{30–33} For example, a 2D van der Waals heterostructure (vdWH) may be more efficient than a single semiconductor as the photocatalyst used for water splitting because the oxidation and reduction reactions of water splitting will take place in different material layers, which will prevent the reverse reaction of water decomposition.\textsuperscript{23} Besides, the valence band offset (VBO) and conduction band offset (VBO) of the vdWH also provide the momentum for the photogenerated holes and electrons, respectively, to remain in perpetual motion, which can prolong their lifetimes. The photoexcitation in photocatalysts of a semiconductor is induced by stimulating the electrons from the VB to the CB, accompanying by Coulomb interaction, which will result in spatial restriction of the electron–hole pairs, named as the exciton. The exciton binding energies ($E_{\text{vb}}$) can quantitate the efficiency of the prevention for recombination of the photogenerated electron–hole pairs, where the higher value of $E_{\text{vb}}$ reveals the more difficult separation of the photogenerated electrons and holes. Some investigations have confirmed that the $E_{\text{vb}}$ of a heterostructure is usually lower than the monolayer materials by GW theory.\textsuperscript{34,35}

Recently, graphene-like gallium nitride (g-GaN) captures considerable attention since it was proposed.\textsuperscript{36} It is a semiconductor with an indirect bandgap,\textsuperscript{7} which can be tuned by chemical modification, stacking structure, or application of an external electric field.\textsuperscript{38,39} Its nanoribbons can potentially be used for spintronics under certain conditions.\textsuperscript{40} Some calculations have been implemented to study the properties of its phonon frequency spectrum, which can prove its stability even at high temperatures.\textsuperscript{41,42} Furthermore, layered g-GaN has been prepared by encapsulated growth using graphene enhanced by migration.\textsuperscript{43} Besides, theoretical predictions suggest that vdWHs based on g-GaN can exhibit novel properties, such as g-GaN/graphene vdWH, which is an n-type Schottky contact, and the transformation from n-type to p-type Schottky contacts can be caused by applying an external electric field.\textsuperscript{44} As for g-GaN/BlueP vdWH, which possesses type-II band alignment, it also has a decent bandgap and band-edge positions utilized as a photocatalyst for water splitting.\textsuperscript{45} By calculating the Gibbs free energy, the g-GaN/Mg(OH)$_2$ vdWH expresses a novel catalytic performance in hydrogen evolution reaction and oxygen evolution reaction for water splitting.\textsuperscript{46} All these investigations suggest that g-GaN can be used in nanoelectronics and optoelectronics.

More recently, another 2D material, monolayered boron selenide (BSe), has been predicted to have thermal stability with an indirect bandgap.\textsuperscript{8} Some heterostructures based on BSe, such as BSe/ZnO and BSe/blue-phosphorene (BSe/BlueP), have also been studied.\textsuperscript{48,49} Interestingly, BSe and g-GaN monolayers possess the same hexagonal atomic structure and similar lattice parameters, denoting that they are compatible components of a vdWH. Here, we investigated the structural, electronic, and optical properties of g-GaN/BSe vdWH using density functional theory (DTF). First, thermal stability of lowest-energy stacking configuration of the heterostructure was determined by ab initio molecular dynamics (AIMD) simulations. Second, the band structure and the band-edge positions of g-GaN/BSe vdWH were calculated. We found that band-edge positions of the g-GaN/BSe vdWH satisfied the energy requirement of oxidation and reduction reactions for water splitting over a wide pH range. The carrier mobility of g-GaN and BSe monolayers as well as the g-GaN/BSe vdWH was also systematically addressed. Then, the interfacial properties of the g-GaN/BSe vdWH, including the charge-density difference and the potential drop, were performed. Finally, in-plane strain was applied to the heterostructure to study how it would tune the optical-absorption ability, the bandgap, and the band-edge position of the heterostructure and how it could improve its performance in water splitting.

## RESULTS AND DISCUSSION

The atomic structures of g-GaN and BSe monolayers are shown in the left panel of Figure 1. The optimized lattice parameters are 3.255 and 3.245 Å for g-GaN and BSe, respectively. The lattice mismatch between g-GaN and BSe is trivial (only 0.31%), indicating that they are good candidate for constructing a heterostructure. The band structures of g-GaN and BSe monolayers are shown in the right panel of Figure 1. The high-symmetry points in BZ are shown in the inset of Figure 1. The high-symmetry points in BZ are shown in the inset of Figure 1. Monolayered g-GaN shows indirect semiconductor characteristics with the CBM located at the Γ point, and the VBM exists at K point (Figure 1a). The gap value is 3.205 eV. Meanwhile, monolayered BSe also exhibits an indirect semiconducting behavior with the VBM located between the Γ and M points, and the VBM appeared at the Γ point (Figure 1b). The gap value is of 3.466 eV. Note that the calculated lattice parameters and the bandgaps of the monolayered g-GaN and BSe are well in agreement with values reported in previous studies.\textsuperscript{37,49}

For the g-GaN/BSe heterostructure, six representative stacking configurations—H$_1$, H$_2$, H$_3$, H$_4$, H$_5$, and H$_6$—were considered; they are illustrated in Figure 2. The binding
energy, distance of the interface, and bond length are calculated for those optimized configurations in Table 1. The most stable stacking configuration of the heterostructure is decided by the lowest $E_b$, which is obtained by $-54.36$ meV/Å$^2$ for the H$_6$ stacking configuration of the g-GaN/BSe heterostructure, suggesting that the g-GaN/BSe heterostructure is formed by vdW interaction. As for the optimized H$_6$ stacking configuration, the interlayer distance ($d_f$) is $3.113$ Å, the bond length of Ga--N and B--Se are calculated to be $1.990$ and $2.188$ Å, respectively. Hereafter, all calculations reported in the paper for the g-GaN/BSe vdWH are based on this stacking configuration.

To further investigate the thermal stability of the g-GaN/BSe vdWH heterostructure, AIMD simulations were performed. A $6 \times 6 \times 1$ supercell of the g-GaN/BSe vdWH was constructed for the AIMD calculations with a Nosé–Hoover heat bath scheme, which contains 216 atoms. As shown in Figure 3a, the AIMD simulations of the g-GaN/BSe vdWH indicates that the atomic structure is still robust within 10 ps at a temperature of 300 K. The fluctuation of temperature and total energy with the simulation step are expressed in Figure 3b, which shows the convergence of results. Therefore, the g-GaN/BSe vdWH is thermally stable at room temperature.

The projected band structure obtained by the HSE06 functional of the g-GaN/BSe vdWH is shown in Figure 4a. Similar to g-GaN and BSe monolayers, the g-GaN/BSe vdWH is still a semiconductor and the bandgap is calculated to be $2.268$ eV. The CBM is dominated by the BSe layer, while the VBM results from the g-GaN layer, suggesting that the

### Table 1. Binding Energy ($E_b$), Distance of the Interface ($d_f$), and Bond Length ($L$) of the Ga--N and B--Se for the ZnO/GaN vdW Heterostructure

| parameter | H$_1$ | H$_2$ | H$_3$ | H$_4$ | H$_5$ | H$_6$ |
|-----------|-------|-------|-------|-------|-------|-------|
| $E_b$ (meV/Å$^2$) | $-43.56$ | $-45.29$ | $-51.03$ | $-45.21$ | $-51.80$ | $-54.36$ |
| $d_f$ (Å) | $3.074$ | $3.804$ | $3.400$ | $3.844$ | $3.337$ | $3.113$ |
| $L_{Ga-N}$ (Å) | $1.990$ | $2.192$ | $1.992$ | $1.993$ | $1.992$ | $1.990$ |
| $L_{B-Se}$ (Å) | $2.189$ | $2.192$ | $2.193$ | $2.193$ | $2.192$ | $2.188$ |

![Figure 2](image-url) Atomic structure of g-GaN/BSe vdWHs with different stacking configurations: (a) H$_1$, (b) H$_2$, (c) H$_3$, (d) H$_4$, (e) H$_5$, and (f) H$_6$. The gray, pale green, green, and orange spheres denote Ga, N, B, and Se atoms, respectively.

![Figure 3](image-url) (a) AIMD snapshots of the structure for the g-GaN/BSe vdWH. (b) The total energy and temperature fluctuation during AIMD simulations at 300 K for the g-GaN/BSe vdWH.
heterostructure has a staggered (type-II) band alignment. To further support this, the band-resolved charge densities of the VBM and the CBM of the g-GaN/BSe vdWH are presented in Figure 4b; they clearly show that the CBM and VBM of the g-GaN/BSe vdWH are mainly donated by the BSe and g-GaN layers, respectively. The VBM mainly results from the s orbital of Ga, while the CBM mainly results from the p orbital of B. When this type-II heterostructure is illuminated by light with the energy of photon larger than the bandgaps of monolayered g-GaN and BSe, the photogenerated electrons will move from the valence band (VB) to the conduction band (CB), then creating holes in the VB (Figure 4c). In addition, the photogenerated electrons tend to migrate from the CB of the g-GaN layer to the CB of the BSe layer owing to the existence of conduction band offset (CBO), whereas the photogenerated holes will migrate from the VB of the BSe layer to that of the g-GaN layer driven by the valence band offset (VBO). The calculated CBO and VBO are 0.155 and 0.348 eV.

**Figure 4.** (a) Projected band structure calculated using the HSE06 functional of g-GaN/BSe vdWH; the red and black dotted lines are the donation of the BSe layer and the g-GaN layer, respectively, the Fermi level is set as zero by the gray dashed line. (b) Band-resolved charge densities; the gray, pale green, green, and orange spheres indicate Ga, N, B, and Se atoms, respectively. (c) Schematic of migration of photogenerated charges at the interface of the g-GaN/BSe vdWH. (d) Band-edge positions of g-GaN and BSe monolayers as well as the g-GaN/BSe vdWH.

**Figure 5.** Transport directions of atomic structures for monolayered (a) g-GaN, (b) BSe, and (c) g-GaN/BSe vdWH; the gray, pale green, green, and orange spheres represent Ga, N, B, and Se atoms, respectively. (d–f) ΔE of orthorhombic monolayered (d) g-GaN, (e) BSe, and (f) g-GaN/BSe vdWH under external strain. (g–i) Band-edge positions of CBM and VBM for monolayered (g) g-GaN, (h) BSe, and (i) g-GaN/BSe vdWH under external strain.
Table 2. Effective Mass ($m^*$), Elastic Modulus (C), Deformation Potential Constant ($E_d$), and Carrier Mobility ($\mu$) of an Electron and a Hole in Monolayered g-GaN, Monolayered BSe, and the g-GaN/BSe vdWH along the Transport Directions Obtained by PBE$^a$

| materials            | direction | carrier | $m^*$ (m_e) | C (N/m) | $E_d$ (eV) | $\mu$ (cm$^2$V$^{-1}$s$^{-1}$) |
|----------------------|-----------|---------|-------------|---------|------------|-------------------------------|
| g-GaN                | $A_1$     | electron| 0.21        | 78      | −10.09     | 287.93                        |
|                      |           | hole    | −1.26       |         | −0.70      | 1741.43                       |
| g-GaN                | $A_2$     | electron| 0.21        | 79      | −9.88      | 304.15                        |
|                      |           | hole    | −1.21       |         | −0.61      | 2395.72                       |
| BSe                  | $A_1$     | electron| 1.38        | 176     | −2.573     | 355.99                        |
|                      |           | hole    | −1.53       |         | −6.200     | 17.01                         |
| g-GaN/BSe            | $A_1$     | electron| 0.15        | 176     | −7.133     | 419.01                        |
|                      |           | hole    | −1.47       |         | −6.100     | 18.25                         |
| g-GaN/BSe            | $A_2$     | electron| 0.17        | 230     | −8.87      | 2207.53                       |
|                      |           | hole    | −2.77       |         | −1.44      | 315.63                        |

$^a$A$_1$ and A$_2$ represent the armchair and zigzag directions, respectively.

The electron and hole mobilities in g-GaN and BSe monolayers as well as the g-GaN/BSe vdWH were also investigated as they are important factors that control the usefulness of the material as a photocatalyst. The two charge-transport directions are armchair (A$_1$) and zigzag (A$_2$) directions, as shown in Figure 5a–c. The response of the energy for the external strain of the monolayered g-GaN and BSe monolayers as well as the g-GaN/BSe vdWH are expressed in Figure 5d,f,h, respectively, which are useful to calculate the elastic modulus for those layered materials. The change in CBM and VBM energy resulting from the external strain for g-GaN and BSe monolayers as well as the g-GaN/BSe vdWH is shown in Figure 5e,g,i, respectively. Table 2 shows the calculated effective mass, elastic modulus, and carrier mobility of g-GaN and BSe monolayers as well as the g-GaN/BSe vdWH at 300 K. The obtained electron mobilities in monolayered g-GaN, BSe, and the g-GaN/BSe vdWH are 287.93, 355.99, and 2207.53 cm$^2$V$^{-1}$s$^{-1}$, respectively, along the armchair direction, while the mobilities are 304.15, 419.01, and 2129.38 cm$^2$V$^{-1}$s$^{-1}$, respectively, along the zigzag direction. Meanwhile, the mobilities of holes in g-GaN and BSe monolayers as well as the g-GaN/BSe vdWH are 1741.43, 17.01, and 315.63 cm$^2$V$^{-1}$s$^{-1}$, respectively, along the armchair direction, and the 2395.72, 18.25, and 306.94 cm$^2$V$^{-1}$s$^{-1}$, respectively, along the zigzag direction.
respectively, along the zigzag direction. One can clearly see that the g-GaN/BSe vdWH can improve the carrier mobility of the monolayered BSe along both the transport directions. Furthermore, when compared with the carrier mobilities in other 2D materials, which can be also used as photocatalysts for water splitting, the values in the g-GaN/BSe vdWH is higher than those in BlueP (1711 cm$^2$V$^{-1}$s$^{-1}$), MoS$_2$ (200.52 cm$^2$V$^{-1}$s$^{-1}$), and WS$_2$ (542.29 cm$^2$V$^{-1}$s$^{-1}$). Therefore, compared with those 2D materials, the g-GaN/BSe vdWH has advantageous ability to promote the photogenerated electron–hole pairs flowing to the surface, which guarantees the occurrence of oxidation and reduction reactions. Therefore, with such a high carrier mobility, the g-GaN/BSe vdWH can reduce the carrier recombination rate to ensure the better photocatalytic performance.

Then, we turn to investigate the interface properties of g-GaN/BSe vdWH. The charge difference ($\Delta \rho$) was calculated by Bader charge analysis. The isosurfaces of charge difference are shown in Figure 6a, and one can clearly see that the g-GaN layer act as an acceptor of 0.0031 lel electrons form the BSe layer. In addition, a large potential drop ($\Delta V$) of 5.712 eV across the interface of the g-GaN/BSe vdWH can be found in Figure 6b, indicating that a strong built-in electric field is generated, which will further cause the separation of photogenerated electron–hole pairs.

The ability to capture a considerable fraction from the spectrum of visible light is a significant requirement for photocatalysts used for water splitting because the visible light spectrum (about 380–800 nm) occupies almost half of the solar spectrum. The optical absorption spectrum for the g-GaN/BSe vdWH is expressed in Figure 7a. The maximum absorption of visible light by the g-GaN/BSe vdWH is 1.470 × 10$^5$ cm at a wavelength of 380 nm, and there is another absorption peak located at 420 nm in the visible light region. The calculated optical absorption of the g-GaN/BSe vdWH indicates that it possesses excellent capacity to capture the visible spectrum. Furthermore, we also apply the biaxial strain on the g-GaN/BSe vdWH to see whether it can further enhance the optical-absorption ability. The results are also shown in Figure 7a. When the heterostructure was subjected to tensile strain values of 1, 2, 3, and 4%, peaks observed at 1.583 × 10$^5$, 1.542 × 10$^5$, 1.502 × 10$^5$, and 1.471 × 10$^5$ cm, respectively, are recorded at wavelengths of 394, 411, 437, and 468 nm, respectively. It is evident that the redshift phenomenon is observed in the spectrum of g-GaN/BSe vdWH and the overlap between the absorption spectrum and the solar flux become larger after the application of a biaxial tensile strain. Therefore, the application of a biaxial tensile strain can enhance the sunlight-absorption ability of the heterostructure. Besides, in the ultraviolet region, there are also some absorption peaks for g-GaN/BSe vdWH, which is even higher than the other reported 2D vdWHs, such as AlN/BP (AIN/ BP Heterostructure Photocatalyst for Water Splitting), g-GaN/BlueP (RSC Adv.), WS$_2$/BSe (WS$_2$/BSe van der Waals type-II heterostructure as a promising water splitting photocatalyst), etc., as a photocatalyst for water splitting.

Using biaxial strain to tune the electronic properties of the 2D heterostructure is also a popular method. The variation of bandgap of the g-GaN/BSe vdWH with tensile strain is shown in Figure 7b. In general, the energy of the CBM quickly decreases when the tensile strain increased to 5%, whereas the energy of the VBM gradually increases with the strain. The band-edge positions of the g-GaN/BSe vdWH remain suitable for the oxidation potential ($O_2/H_2O$) and reduction potential ($H^+/H_2$) at pH 0 and 7 for water splitting under strain strengths of 1 and 2%. When the tensile strain with strengths of 3 or 4% is applied, the g-GaN/BSe vdWH can decompose water into $H_2$ and $O_2$ at pH 0. Therefore, the applied tensile strain not only increases the sunlight-absorption ability of the heterostructure but also retains its application in photocatalysts for water splitting in a certain region.

**CONCLUSIONS**

The structural, electronic, interfacial, and optical properties of the g-GaN/BSe vdWH were explored by DFT calculations. The most stable configuration of the g-GaN/BSe vdWH was obtained with a binding energy of $-54.36$ meV/A$^2$, which is proved to be thermally stable at room temperature by AIMD simulations. The g-GaN/BSe vdWH is an indirect semiconductor with a gap value of 2.268 eV. It also possesses a type-II band alignment, which can prevent recombination of the photogenerated electrons and holes. The band-edge positions of the g-GaN/BSe vdWH show that the heterostructure has suitable band edges for the redox potential of water splitting at pH 0 and 7. Then, the high carrier mobility was found in the g-GaN/BSe vdWH that the mobility for electrons are 2207.53 and 2129.38 cm$^2$V$^{-1}$s$^{-1}$ along armchair and zigzag directions, respectively. The hole mobilities for the g-GaN/BSe vdWH are 315.63 and 306.94 cm$^2$V$^{-1}$s$^{-1}$ along the armchair and zigzag directions, respectively. Furthermore, the formation of a large in-built electric field was found at the interface, which can also promote the separation of photo-
generated charges. Moreover, the g-GaN/BSe vdWH shows excellent absorption ability for sunlight, which can also be effectively enhanced by a biaxial tensile strain. These findings suggest the promising role of g-GaN/BSe vdWH as a high-efficiency photocatalyst to decompose water for hydrogen production. Our work is also expected to offer guidelines for the design of other heterostructures based on g-GaN or BSe as photocatalysts for water splitting.

**METHODOLOGY**

In this research, all simulations were carried out by first-principles calculations using the Vienna Ab initio Simulation Package (VASP)\(^1\) based on density functional theory. The Perdew–Burke–Ernzerhof (PBE) functional\(^2\) based on generalized gradient approximation (GGA) was implemented for the exchange correlation functional. The hybrid Heyd–Scuseria–Ernzerhof (HSE06) functional was also utilized for more accurate bandgap calculations. A relatively large 550 eV plan-wave cutoff was used to guarantee the accuracy of calculations. The first Brillouin zone (BZ) was sampled by Monkhorst–Pack \(k\)-point mesh with a grid of 17 \(\times\) 17 \(\times\) 1 in reciprocal space. The vacuum slab is 20 Å, which can effectively reduce interactions between adjacent atomic layers. All the structures were fully relaxed until the Hellmann–Feynman force on each atom is smaller than 0.01 eV Å\(^{-1}\). Besides, the convergence range for each energy was set to less than 1 \(\times\) 10\(^{-3}\) eV. In addition, weak dispersion forces were corrected by using the DFT-D3 method of Grimme,\(^3\) and dipole corrections were also considered in all of the calculations.

The binding energy (\(E_b\)) was calculated as follows

\[
E_b = E_{g-GaN/BSe} - E_{g-GaN} - E_{BSe}
\]  
(1)

where \(E_{g-GaN/BSe}\), \(E_{g-GaN}\), and \(E_{BSe}\) represent the total energy of the g-GaN/BSe vdWH, g-GaN monolayer, and BSe monolayer, respectively.

The charge-density difference (\(\Delta \rho\)) was calculated by

\[
\Delta \rho = \rho_{g-GaN/BSe} - \rho_{g-GaN} - \rho_{BSe}
\]  
(2)

where \(\rho_{g-GaN/BSe}\), \(\rho_{g-GaN}\), and \(\rho_{BSe}\) are the total charge density of the g-GaN/BSe vdWH, g-GaN monolayer, and BSe monolayer, respectively.

The carrier mobility of each of the 2D materials (\(\mu_{2D}\)) was decided by the deformation potential theory\(^4\)

\[
\mu_{2D} = \frac{e\hbar^2 C_{2D}}{k_BT m^* m_i \rho_i}\n\]  
(3)

where \(e\) is the charge of an electron, \(\hbar\) is the reduced Planck's constant, \(k_B\) is the Boltzmann constant, \(T\) is the temperature, \(m^*\) is the effective mass along the transport direction, and \(m_i\) is the average effective mass, which was calculated using \(m_i = \sqrt{m_{\|} m_{\perp}}\). The deformation potential constant (\(\rho_i\)) of the electron in the CBM and the hole in the VBM along the transport direction is expressed as \(\rho_i = \Delta V_i/(\Delta l/l_0)\), where \(\Delta V_i\) is the energy difference between the CBM and VBM under an applied strain in the range of −0.5 to 0.5%, \(l_0\) is the lattice parameter, and \(\Delta l\) is the deformation of \(l\) by strain. The elastic modulus of the 2D material (\(C_{2D}\)) is defined as \(C_{2D} = [\partial^2 E/\partial \Delta l^2]/\rho_i\), where \(E\) is the energy difference compared with the unstrained 2D system, \(l\) is the applied strain, and \(S_0\) is the lattice volume of the 2D system at equilibrium.

The absorption coefficient was obtained using the equation\(^5\)

\[
\alpha(\omega) = \frac{\sqrt{2\alpha}}{c} \cdot [\varepsilon_1(\omega) + \varepsilon_2(\omega)]^{1/2} - \varepsilon_1(\omega)^{1/2}
\]  
(4)

where \(\varepsilon_1(\omega)\) and \(\varepsilon_2(\omega)\) are used for the real and imaginary parts of the dielectric constant, respectively. Moreover, \(\omega\), \(\alpha\), and \(c\) express the angular frequency, absorption coefficient, and the speed of light in vacuum, respectively.

**AUTHOR INFORMATION**

**Corresponding Authors**

*E-mail: tangwc@seu.edu.cn (W.T.).
*E-mail: mingleisun@outlook.com (M.S.).

**ORCID**

Yi Luo: 0000-0002-2548-1758
Jyh-Pin Chou: 0000-0001-8336-6793
Minglei Sun: 0000-0001-5105-0065

**Notes**

The authors declare no competing financial interest.

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