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Investigation of Photocatalytic Performance of GaN-WSSe Under Vertical Strain

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ABSTRACT

The utilization of mechanical strain is an essential way to modify and optimize the physical properties of materials, possibly making them usable for a variety of applications, including nanoelectronics and renewable energy sources. Hydrogen production through water splitting (has been proposed as a promising solution to the today's global energy crisis. Therefore, there is a great demand for exploring low-cost and efficient photocatalysts for this process. We studied the electronic and structural properties, and band alignment of WSSe/graphene-like GaN (g-GaN) heterostructure. Our results reveal that the band alignment of the AA-stacked WSSe/g-GaN heterostructure satisfies the water redox potentials at a pH of 7. In order to investigate the effect of regulation on these two heterostructures, out of plane strain ranging from -2% to 2% is utilized. The results demonstrate that adding strain will improve the photocatalytic characteristics notably, which were assessed depending on the valence and conduction band edge potentials.

Keywords: vdW heterostructures, Photocatalytic performance, Density functional theory, Electronic properties

GaN-WSSe'nin Dikey Gerinim Altında Fotokatalitik Performansının İncelenmesi

ÖZ

Mekanik gerinim uygulaması, malzemelerin fiziksel özelliklerini ayarlamak ve optimize etmek için çok önemli bir tekniktir. Bu uygulama sayesinde malzemeler yenilenebilir enerji kaynakları ve nanoelektronik dahil olmak üzere çeşitli uygulamalar için potansiyel olarak yararlı olmaktadır. Su ayırma yoluyla hidrojen üretimi, enerji krizine umut verici bir çözüm olarak önerilmektedir. Bu nedenle, bu işlem için düşük maliyetli ve verimli fotokatalizörlerin keşfedilmesi için literatürde büyük ölçüde talep bulunmaktadır. Bu çalışmada WSSe/grafen benzeri GaN (g-GaN) heteroyapısının elektronik özellikleri, yapısal özellikleri ve bant hizalaması araştırılmıştır. Sonuçlarımız, AA yığınlı WSSe/g-GaN heteroyapısının bant hizalamasının, pH7'de su redoks potansiyellerini karşıladığını ortaya koymaktadır. Düzenlemenin bu iki heteroyapı üzerindeki etkisini araştırmak için %-2 ile %2 arasında değişen düzlem dışı gerinim uygulanmıştır. Sonuçlar heteroyapıya gerinim uygulanmasının değerlik ve iletim bandlarının redoks potansiyellerine göre sıralanması ile fotokatalitik özelliklerin artıracağını göstermektedir.

Anahtar Kelimeler: vdW heteroyapıları, Fotokatalitik performans, Yoğunluk fonksiyonel teorisi, Elektronik özellikler

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1. Introduction

The world needs to create renewable and ecologically friendly energy supplies due to the major energy and environmental issues that have arisen in recent years as an outcome of the scarcity of fossil fuels. Among renewable energy sources solar energy is one of the most abundant, cost-effective, and ecologically friendly renewable energy sources. One method for converting solar energy is to produce hydrogen by the photocatalytic water splitting of water. Because of its high energy density (120 MJ/kg), abundance, and clean combustion, hydrogen is expected to be a popular fuel in the coming decades. Therefore, researchers are urged to use semiconducting materials for hydrogen production and water splitting because there is a plentiful supply of both these resources (Fox and Dulay,1993; Hoffmann et al., 1995; Linic et al., 2011; Christooforidiis and Fornasiero, 2017). By converting solar energy into chemical hydrogen energy, solar-driven photocatalytic water splitting has become recognized as a realistic and sustainable, ecologically friendly, and cost-effective solution to the world's enormous energy and environmental concerns. For commercial applications, photocatalysts with a visible light absorption range, high catalytic efficiency, robust redox ability, and long-term stability are required. Nevertheless, contemporary single semiconductors cannot achieve all of the aforementioned needs since increasing photoabsorption demands a high band gap, which limits light-harvesting range, while boosting redox ability demands a narrow band gap, which inevitably results in poor redox ability. Numerous researchers claim in the literature that the most promising materials for water splitting are 2D materials with exceptional and superior properties (such as electrical, mechanical, and optical etc.) when in contrast with 3D bulk materials due to the phenomenon of quantum confinement in the axial direction of thickness of the atomic layer. In addition to having an acceptable band structure, least carrier recombination, and an outstanding visible-light absorption coefficient, high-efficiency photocatalytic materials must remain robust over an extended period. As a result, the majority of 2D materials must be modified to work satisfactorily as photocatalysts for water splitting. To further enhance the performance of 2D materials, van der Waals (vdW) heterostructures can be built by stacking numerous 2D crystals on top of each other. These heterostructures may have new or improved photoelectric properties while retaining the initial features of isolated monolayers (Novoselov et al., 2016; Zeng et al., 2021; Yu et al., 2022; Song et al., 2021; He et al., 2022). Because of their remarkable properties, such as potent light-matter interaction, spin-valley locking effects, attractive catalytic activity, greater carrier mobility, and an enormous surface area, transition metal dichalcogenides (TMDCs) are the most promising 2D materials, especially in the field of photocatalytic water splitting (Andoshe et al., 2015; Hsieh et al., 2017; Brennan et al., 2017; Eda et al., 2011; Wang et al., 2015; Wang et al., 2012). Monolayer Janus TMDs with unique chalcogen ions on opposing sides of the monolayer and the chemical formula MXY (M = Mo, W; X, Y = S, Se, Te) can provide a pure polar surface (Yao et al., 2017). Even though polar surfaces are typically unstable, a single layer Janus TMDs have been successfully produced using a modified chemical vapor deposition approach (Yao et al., 2017; Riis-Jensen et al., 2018). These materials also have novel properties such as Rashba splitting and piezoelectricity. The inherent dipole moment of Janus TMDs has been discovered to assist spatially segregate excited carriers and lengthen the recombination of carriers time by orders of magnitude when contrasting with standard MX_2 TMDs (Lu et al., 2017; Zhang et al., 2017; Liang et al., 2018). Furthermore, it is also demonstrated that TMDs including Se or Te have greater aqueous durability in comparison to those containing only S. As a result, in photocatalytic or other kinds of light capturing applications, Janus TMDs may outperform typical TMDs (Long et al., 2019). WSSe, like MoSSe, has been stated, and it differs from WS_2 and WSe_2 owing to its electrical nature and structural differences. The direct bandgap semiconductor with fascinating optical features observed in the ultrathin Janus

WSSe layer is appropriate for use in photovoltaics (Guan et al., 2018). Further, WSSe outperforms other transition metal dichalcogenides (TMD)-based photocatalytic water splitting catalysts (Er et al., 2018). Additionally, in different applications areas, the WSSe-based FET has a high current on/off ratio and high charge mobilities when compared to other TMD-based conventional field effect transistors (FETs) (Karande et al., 2016). For solar cell applications, bilayer WSSe exhibits enhanced photoelectric conversion (Zhou et al., 2019). Therefore, these improvements encourage researchers to dig deeper into the heterostructures of Janus WSSe materials. Heterostructures allow for effective tuning of the position and band gap width for the need of a photocatalyst. Because hydrogen and oxygen are produced at distinct levels of the materials, Type-II heterostructures offer great opportunities for water splitting. GaN has drawn more attention from researchers due of its strong thermal conductivity and thermal stability (Neumayer and Ekerdt, 1996; Liao et al., 2014; Zhang et al., 2014). The present study focuses on four vdW heterostructures using g-GaN and Janus-WSSe monolayers. Our investigation, carried out through density-functional theory (DFT) computations, aims to examine the structural, electronic, and photocatalytic properties of these heterostructures, including the impact of out of plane uniaxial strain on their properties. Our study confirms that the tuneability of the band gaps and band alignment of these heterostructures with the help of out of plane strain. Also, the comparison of the photocatalytic properties of these structures in both strained and unstrained conditions are presented.

2. Method

In this paper, the Quantum Espresso software was used to perform all density functional theory (DFT) calculations utilizing DFT on a plane-wave basis. To characterize the electron-ion interaction, we used norm conserving pseudo-potentials, which are more accurate than the ultra-soft pseudo-potentials. The exchange-correlation relationship was explained using the Perdew-Burke-Ernzerhof (PBE) functional within the generalized gradient approximation (GGA). The DFT-D3 approach was used to include the contribution from the van der Waals (vdW) interaction between layers. Spin-orbit coupling (SOC) was also taken into account in self consistent calculations using the fully relativistic norm preserving pseudo-potentials. The plane wave expansion's kinetic energy cutoff was set at 100 Ha. Integrations over the Brillouin zone (BZ) were performed using a 24x24x1 Monkhorst-Pack k-point mesh for a perfect supercell. To prevent interactions in the stacking direction between repeated slabs, a vacuum layer thickness of 25 Å was added. All structures were relaxed until the Hellmann-Feynman forces on every atom were less than 0.01 eV/A, while the total energy convergence was below 10 eV.

3. Results and Discussion

To gain comprehensive knowledge of the stacking of graphene-like GaN (g-GaN) and Janus-WSSe in van der Waals heterostructures, we initially examined the structural and electronic properties of the individual monolayers. The lattice parameters and Ga-N bond length of the g-GaN monolayer were found to be 3.237 Å and 1.869 Å, respectively. As depicted in Fig. 1 (a), g-GaN displays an indirect band gap of 2.234 eV with the CBM and VBM situated at the **K** point and **Γ** point in the Brillouin zone, respectively. Our findings are consistent with previous investigations (Mu, 2015; Xu et al., 2013). In the case of the Janus-WSSe (or WSSe) monolayer, the lattice parameters and bond lengths of W-S and W-Se were determined to be 3.251 Å, 2.434 Å, and 2.551 Å, respectively. The Janus-WSSe (or WSSe) band structure in Fig. 1 (b) additionally reveals that it is a 1.433 eV direct-gap semiconductor with both the conduction band minimum (CBM) and the valence band maximum (VBM) positioned near the **K** point in the Brillouin zone. Our findings show that the Janus-WSSe (or WSeS) monolayer's lattice properties and bandgap are comparable to those of WS_2 (3.18 Å, 2.38 eV) (Chang et al., 2013; Wang et al., 2015) and WSe_2 (3.32 Å, 2.11 eV) (Chang et al.,

2013; Wang et al., 2015), supporting the credibility of this study.

The g-GaN and Janus-WSSe (or WSeS) monolayers have a lattice mismatch of less than 1%, indicating that their heterostructures may be formed with minimum lattice distortion and a decreased risk of defects. It is feasible to use of their 1x1 primitive cells. The g-GaN/Janus-WSeS and g-GaN/Janus-WSSe structures are named based on the relative positions of the Se and S atoms with respect to g-GaN, with the former resulting from the closer proximity of Se atoms to g-GaN and the latter from the closer proximity of S atoms to g-GaN. In this study, we have explored the most common stacking configurations, namely AA and AB, for both g-GaN/Janus-WSeS and g-GaN/Janus-WSSe. Figure 2 depicts the various stacking arrangements for g-GaN/Janus-WSeS heterostructures.

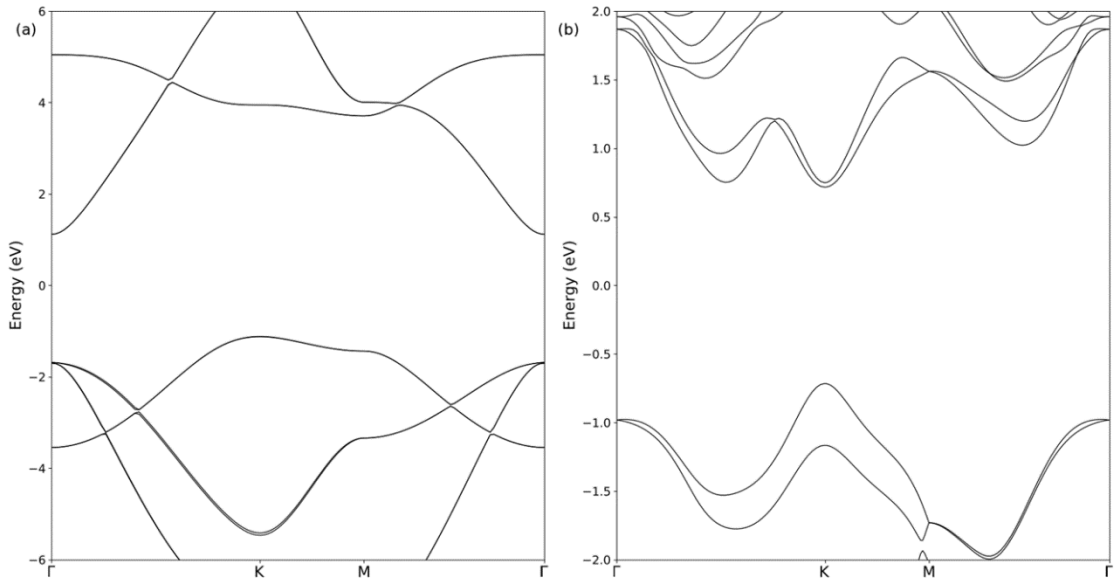

Figure 1. The electronic band structure of (a) monolayer g-GaN and (b) WSSe including spin-orbit coupling (SOC). The Fermi level is set to zero energy level.

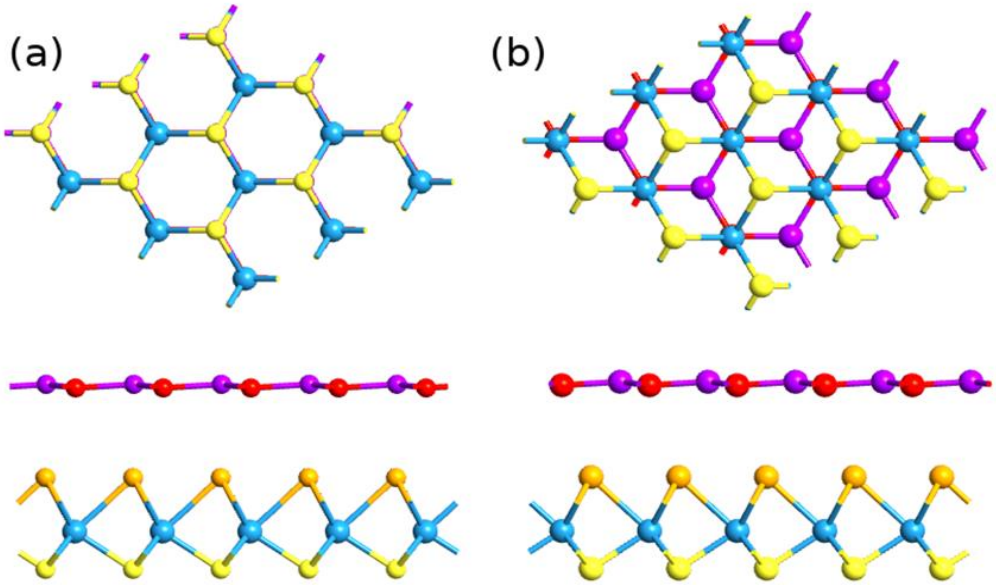

Figure 2. WSSe/GaN vdW heterostructure top and side views with different stacking implementations: (a) WSSe/GaN (AA-stacking) and (b) WSSe/GaN (AB-stacking).

In order to measure the intensity of the interaction quantitatively, we computed the binding energies (E_b) per unit cell using the following equation of

$$E_b = E_{\mathrm{WSSe/GaN}} - E_{\mathrm{GaN}} - E_{\mathrm{WSSe}} \quad . \qquad \textbf{(1)}$$

Here, $\boldsymbol{E}_{\mathrm{WSSe/GaN}}$, $\boldsymbol{E}_{\mathrm{GaN}}$, and $\boldsymbol{E}_{\mathrm{WSSe}}$ correspond to the total energy of the WSSe/GaN heterostructure, monolayer g-GaN, and monolayer WSSe, respectively. Essentially, we assessed the stability of various configurations for WSSe/g-GaN heterostrcutrues using the binding energy. We calculated binding energies of 88 meV/atom and 71 meV/atom with the interlayer distances of 3.081 Å and 3.095 Å for AA- and AB- stacked WSeS/g-GaN heterostructures, respectively. Similarly, the binding energies of 77 meV/atom and 73 meV/atom with the interlayer distance of 2.955 Å and 3.019 Å for AA- and AB-stacked WSSe/g-GaN heterostructures are calculated, respectively. These results are a common characteristic of vdW bonded systems, such as graphite (which has a distance of 3.3 Å). The negative and small interface binding energies suggest that the inter-layer couplings belong to vdW interaction, and their arrangements are energetically favorable. Therefore, the 2D hetero bilayers exhibit weak interactions via vdW interaction. According to binding and relaxation energies, the AA-stacked WSeS/g-GaN heterostructure is the most robust of these stacked heterostructures. As a result, we solely used this structure in the subsequent computations.

Figure 3 (a) shows the electronic structure of AA-stacked WSeS/g-GaN heterostructure, computed employing PBE functional. It is clear that the WSeS/g-GaN heterostructure is a direct semiconductor with the band gap of 1.485 eV which is comparable with the previous work (Idrees et al., 2020). The VBM and CBM are located at **K** point in the Brillouin zone. Next, to analyze the atomic contributions to VBM and CBM, Figure 3 (b) displays the calculated partial density of states (PDOS). The main contributions to the VBM and CBM are included for the sake of clarity. The results show that, across all the systems, the N p orbitals of GaN are the primary contributors to the VBM. Conversely, the W d orbitals of WSSe account for the main contributions to the CBM. As a result, the CBM and VBM are situated on opposite sides of the heterostructure, resulting in a type-II band alignment.

Stretching two-dimensional materials can be accomplished in various kinds of methods, including employing an adaptable substrate that can be flexed a piezoelectric substrate that may have its size modified by an electric field, or exposing the material to a network of nanopillars. The present study has been devoted to exploring the impact of out of plane uniaxial strain on the electronic and photocatalytic properties of WSeS/GaN heterostructure. The investigation has been conducted by maintaining a uniform 2% strain gap under both compressive and tensile strain. Figure 4 displays the band structure of the strained WSeS/GaN heterostructure with the different strain strengths -1%, -2%, 1%, and 2%, respectively. Here positive strain values imply tensile strain, while negative strain values indicate compressive strain. It is found that the band gap of the WSeS/GaN heterostructure can be modulated with the application of strain while the band gap nature remains direct. The band gap is decreased with the tensile out of plane uniaxial strain by ~6 meV while it is increased by 7 meV with the compressional out of plane uniaxial strain.

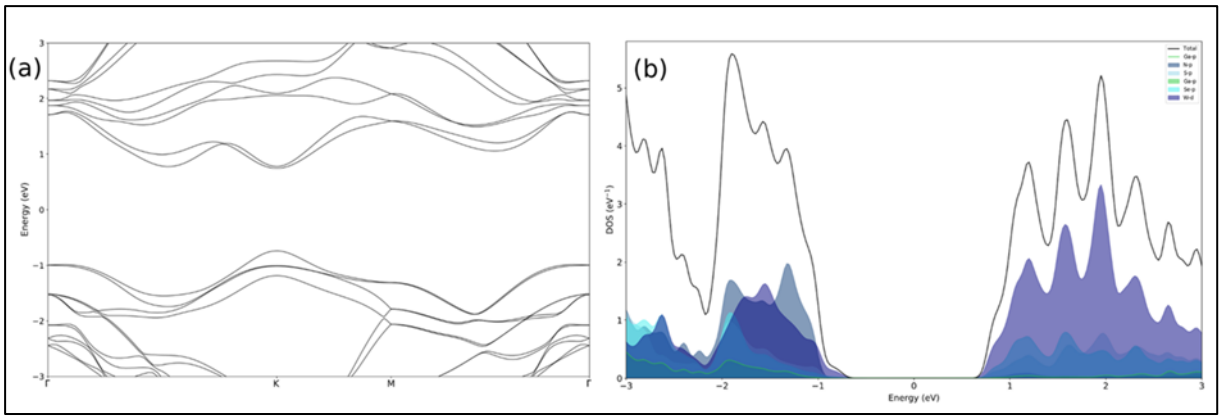

Figure 1. (a) Electronic structure and (b) partial density of states of AA-stacked WSeS/g-GaN heterostructure. The Fermi level is set to zero.

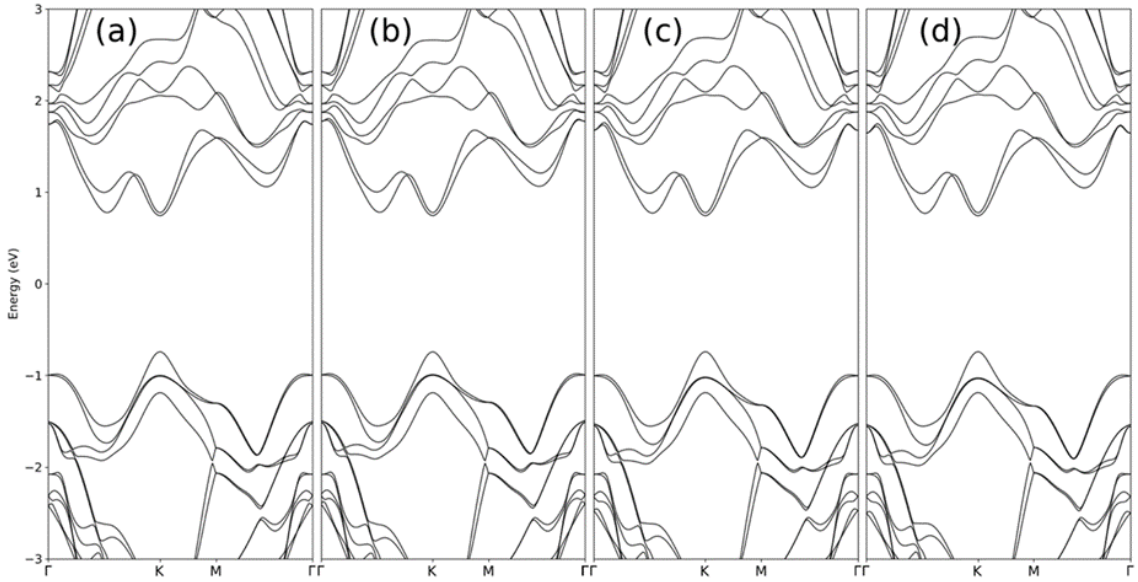

Figure 2. Band structure of AA-stacked WSeS/g-GaN heterostructure under out-of-plane uniaxial strain of (a) -1%, (b) -2%, (c) 1%, and (d) 2%. The Fermi level is set to zero.

To enable effective water splitting, a photocatalyst must have its band edge overlapping with the oxidation and reduction potentials. The band boundaries of an AA-stacking WSeS/g-GaN heterostructure relative to the vacuum level are shown in Figure 5. At pH 7, the conduction band minimum (CBM) of the AA-stacking WSeS/g-GaN heterostructure is positioned at a higher energy level than that of H^+/H_2 (-4.027 eV), while its valence band minimum (VBM) is situated at a lower energy level than that of O_2/H_2O (5.257 eV). This arrangement indicates that the heterostructure possesses a favorable band edge alignment for photocatalytic water splitting at pH 7, where water is in equilibrium with H^+/H_2 and O_2/H_2O. Therefore, the AA-stacking WSeS/g-GaN heterostructure shows promise as an efficient photocatalyst for this purpose with a high catalytic efficiency. According to Fig. 5, this heterostructure may be employed as a high-performance photocatalyst that produces up to 2% out of plane strain. However, at out of plane compressive strain of 2% it is not suitable for reduction but is for oxidation. These results suggest that this out of plane strain method is a promising technique to produce clean and renewable energy device applications.

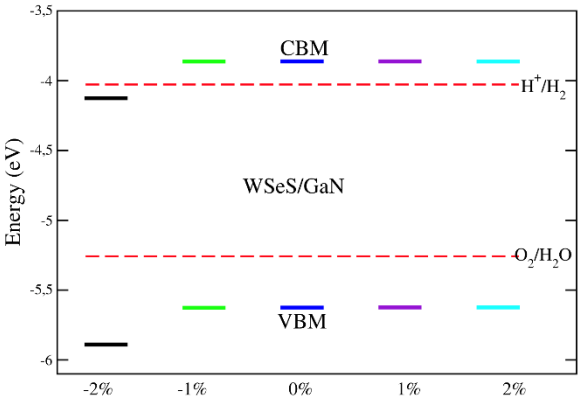

Figure 3. The redox potential of water separation at pH 7, as well as the conduction band and valence band orientation of the AA-stacking WSeS/g-GaN vdW heterostructure, are highlighted for comparison.

4. Conclusion

In overall, we explored four WSeS/g-GaN vdW heterostructures. Among these, we found the AA-stacking WSeS/g-GaN heterostructure as the most stable ones. The structural, electrical, and photocatalytic features of this vdW heterostructure were thereafter theoretically examined via first principal computations in accordance with density functional theory. Our results show that the AA-stacking WSeS/g-GaN heterostructure is direct semiconductor with an intrinsic type-II band alignment. Furthermore, we applied out of plane uniaxial strain to this vdW heterostructure to tune electronic properties. The band nature remained unchanged when both tensile and compressional strain was applied. The photocatalytic behavior exhibited by this vdW heterostructure verifies the potential of WSeS-g-GaN for efficient photocatalytic water splitting at pH 7, both without strain and under tensile and compressional strain of up to 2%.

Author Contributions

Ö. C. Yelgel: Conceptualization, Data Curation; Formal Analysis, Investigation, Methodology, Project Administration, Resources, Software, Supervision, Validation, Visualization, Roles/Writing-Original Draft; Writing - Review & Editing.

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