Band Alignments of Ternary Wurtzite and Zincblende III-Nitrides Investigated by Hybrid Density Functional Theory

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ABSTRACT: Band gaps and electron affinities of binary and ternary, wurtzite (wz-) and zincblende (zb-) III-nitrides are investigated using a unified hybrid density functional theory, and band offsets between wz- and zb- alloys are calculated using Anderson’s electron affinity model. A conduction (and valence) band offset of 1.85 (0.89) eV has been calculated for zb-GaN/InN heterojunctions, which is 0.25 eV larger (and 0.26 eV smaller) than that of the wz- counterpart. Such polarization-free zb-GaN/InGaN/GaN quantum well structures with large conduction band offsets have the potential to suppress electron leakage current and quantum-confined Stark effects (QCSEs). Contrarily, the conduction (and valence) band offset of zb-AlN/GaN heterojunctions is calculated to be 1.32 (0.43) eV, which is 1.15 eV smaller (and 0.13 eV larger) than that of the wz- case. The significant reduction in zb-AlN/GaN band offsets is ascribed to the smaller and indirect band gap of zb-AlN—the direct-to-indirect crossover point in zb-Al1XGa1−XN is when X ~ 65%. The small band gap of the zb-AlN barrier and the small conduction band offsets imply that electrons can be injected into zb-AlN/GaN/AlN quantum well heterostructures with small bias and less energy loss when captured by the quantum wells, respectively, i.e., loss as heat is reduced. The band gap of ternary III-nitrides does not linearly depend on alloy compositions, implying a nonlinear dependence of band offsets on compositions. As a result, the large bowing of the conduction band offset is identified and ascribed to the cation-like behavior of the conduction band minimum, while the linear dependence of the valence band offset on compositions is attributed to the anion-like character of the valence band maximum.

I. INTRODUCTION

III-nitrides (i.e., AlGaInN) have been instrumental in enabling ultraviolet and blue light-emitting diodes (LEDs), high-frequency high-electron-mobility transistors (HEMTs), and negative electron affinity photocathodes. These devices rely on quantum structures or buffer layers composed of heterointerfaces. For instance, blue LEDs utilize GaN/InGaN/GaN quantum well heterostructures to increase the electron-hole spatial overlap for high emission efficiency, and HEMTs utilize AlGaN/GaN heterojunctions to form a two-dimensional electron gas channel for high-speed transport. These devices utilize the conventional wurtzite (wz-) phase of the III-nitrides that comes with challenges. For instance, extending the LED spectrum from blue to green for the use of green LEDs in white light generation has been challenging as inherent spontaneous and piezoelectric polarization in wz- III-nitrides cause the electron-hole spatial separation in quantum wells (i.e., quantum-confined Stark effect (QCSE)) to limit the radiative efficiency. On the electronics side, the inherent spontaneous and piezoelectric polarization in wz- III-nitrides cause HEMTs to be normally on at all times, creating safety concerns in power electronics applications. Zincblende (zb-) III-nitrides offer a solution to overcome these challenges as they are free of both spontaneous and piezoelectric polarization (in the (001) growth direction) thanks to the centrosymmetric crystal structure while having similar benefits.
the band structures (such as the hybrid density functional theory, the \( k \cdot p \) perturbation theory, and the tight-binding model) and (ii) energy references (such as the vacuum level, average electrostatic potentials, charge neutrality levels, and branch-point energies).  

It is important to note that band alignments procured without the impact of strain are known as natural or unstrained band alignments, which are essential to determine the band alignments under a certain strain condition by incorporating deformation potentials. In this work, a unified hybrid functional is introduced to determine band gaps and electron affinities of unstrained binary and ternary, wz- and zb- III-nitrides. The advantage of using the unified approach is that method accuracy is verified by the reported data on wz- III-nitrides, which enables calculating the electronic properties of zb- III-nitrides with high reliability. Electron affinities are calculated based on nonpolar wz- (1010) and zb- (110) planes because earlier works show that interface orientations of (100), (110), and (111) have minor impacts on valence band offsets. Band alignments of binary and ternary, wz- and zb- III-nitrides are derived from band gaps and electron affinities using Anderson’s electron affinity model.

II. RESULTS AND DISCUSSION

Figure 1a shows the electron affinity of binary and ternary III-nitrides. The x-axis labels the alloys ranging from InN and GaN to AlN, while the y-axis is the electron affinity. The black solid line and red dashed line indicate the (1010) facet of wz-alloys and the (110) facet of zb-alloys, respectively. Qualitatively, the electron affinity of III-nitrides on the wz-(1010) and zb-(110) facets has the analogous composition-dependent relation, which reaches the maximum at InN regardless of wz- and zb- crystals and decreases with respect to the increasing mole fraction of Al and Ga. The electron affinity of the wz- alloys reaches the minimum at AlN, while the electron affinity of the zb- alloys reaches the minimum around A\(_{0.75}\)Ga\(_{0.25}\)N because the conduction band minimum shifts from \( \Gamma \)- to X-valley, which will be explained later in light of the band alignments. Quantitatively, the electron affinity of 3.92 eV is obtained on the (1010) facet of wz-GaN, which agrees with 4.06 ± 0.07 eV measured on the same facet. It is worth noting that the electron affinity of 2.6–3.8 eV had been widely reported on the polar (0001) facet of wz-GaN. The reduction of the electron affinity is attributed to the presence of surface adsorption and surface polarity. For instance, the electron affinities of Ga- and N-polar GaN surfaces have been reported to be 3.8 and 3.3 eV, respectively. Experiments and recent generalized gradient approximation (GGA)-based simulations reveal that the electron concentration accumulated around the Ga- and N-dangling bonds at the GaN surface is too low to screen the spontaneous polarization-induced electric field. Consequently, the spontaneous polarization-induced electric field causes an upward surface band bending and leads to the reduction of electron affinity. The calculated electron affinity of wz-AlN is 1.45 eV, which falls within the experimental values ranging from 0.25 ± 0.3 to 1.9 eV. Notably, the large uncertainty is ascribed to the chemically active surface of AlN that is vulnerable to oxygen contamination. For the electron affinity of wz-InN, the measured range of 5.5–5.8 eV is deduced by the conduction band offset of the wz-GaN/InN heterojunction and the electron affinity of wz-GaN, which are consistent with the theoretical values of 5.3 (In-polar c-plane)—5.8 (m-plane) eV using the GW calculation. Our Heyd–Scuseria–Ernzerhof (HSE06) approach procures 5.51 eV for the electron affinity of wz-InN, which is in agreement with the experiments and the more advanced theory.

The electron affinity is sensitive to the atomic arrangement on the surface. wz- crystal structure has two distinct point bases; therefore, the unit cell used to build m-plane slabs involves two asymmetric cation–anion bonds. Since the slabs are generated by repeating the unit cell along the z-axis, two distinct cation bases lead to different surface stoichiometries for ternary wz- III-nitrides. If two different types of cations are involved in the slab, one type of the cations can lie either on the surface layer (type-I cation arrangement) or one atomic layer below the surface layer (type-II cation arrangement), as shown in Figure 1b,c, respectively. The asymmetric cation arrangements in the slab lead to different electron distributions, electrostatic potentials, and dipole moments, which render the surface band bending and the diminution of electron affinity. Consequently, each ternary wz- III-nitride with 25 and 75% alloying ends in two distinct electron affinities depending on the surface stoichiometry represented by the error bars in Figure 1. For example, the electron affinities of wz-In\(_{0.25}\)Ga\(_{0.75}\)N are 5.52 (surface terminates with an In–N bond) and 5.14 eV (surface terminates with a Ga–N bond). Table 1 tabulates the magnitude of the electron affinity and estimated dipole moments for the type-I and type-II cation arrangements. It proves that two different dipole moments are induced by the asymmetric surface stoichiometries. The amplitude of the electron affinity variation is small when the dipole moments are weak. The variation of the electron affinity directly contributes to the variation of band alignments.

| Table 1. Electron Affinities and Estimated Dipole Moments of 25- and 75%-Alloying wz- III-Nitrides for Type-I and Type-II Cation Arrangements |
|------------------|-----------------|-----------------|-----------------|
| alloy            | electron affinity (eV) | dipole moment (type-I) (D) | dipole moment (type-II) (D) |
| A\(_{0.25}\)Ga\(_{0.75}\)N | 3.396 ± 0.048 | 0.084 | 0.018 |
| A\(_{0.75}\)Ga\(_{0.25}\)N | 2.212 ± 0.065 | 0.095 | 0.036 |
| A\(_{0.25}\)In\(_{0.75}\)N | 4.967 ± 0.203 | 0.399 | 0.351 |
| A\(_{0.75}\)In\(_{0.25}\)N | 3.300 ± 0.167 | 0.430 | 0.269 |
| In\(_{0.25}\)Ga\(_{0.75}\)N | 4.624 ± 0.225 | 0.421 | 0.182 |
| In\(_{0.75}\)Ga\(_{0.25}\)N | 5.334 ± 0.191 | 0.273 | 0.663 |

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Therefore, the average value of electron affinities is exploited for band alignments, as shown in Figure 2.

According to Anderson’s electron affinity model, the band diagram of III-nitrides can be aligned with respect to the vacuum energy using the electron affinity and the band gap obtained from the density functional theory (DFT) calculations. Figure 2 summarizes the conduction ($E_c$) and valence ($E_v$) band offsets of wz-GaN, AlGaN, and AlInN indicated by the black solid line and red dashed line, respectively. Instead of using the vacuum energy as a reference level, the band edges are shifted relative to the valence band edge of wz-GaN for convenience. The conduction and valence band offsets between arbitrary two materials can be determined by the difference of $E_c$ and $E_v$ respectively. As a result, the wz- alloys exhibit type-I band alignments, where the conduction (and valence) band offsets of wz-GaN/InN, wz-AlGaN, and wz-AlInN heterojunctions are 1.60 (1.15), 2.47 (0.30), and 4.07 (1.45) eV, leading to the ratios of conduction band offsets to band-gap differences of 0.68, 0.75, and 0.71, respectively. Before further exploration, it is important to validate the accuracy of the methodology through experimental measurements. To begin with, the valence band offset of 1.05 ± 0.25 eV has been probed experimentally for wz-GaN/InN heterojunctions, which is in agreement with our simulation result of 1.15 eV. On the other hand, the calculated valence band offset of the wz-AlN/GaN heterostructure (0.3 eV) is consistent with the X-ray photoemission spectroscopy measurement of 0.3 ± 0.1 eV, while, for wz-AlInN/InN heterostructures, the calculated valence band offset of 1.45 eV agrees with the X-ray photoemission spectroscopy measurement of 1.4 ± 0.1 eV. Notably, the deviation between the experiment and simulation and the uncertainty in experiments are ascribed to the variation of defectivity, strain, stoichiometry, surface polarity, and the chemical potency of reference core levels. Based on the validated methodology, the band alignments of zb- III-nitrides are calculated. Figure 3 demonstrates the conduction (black solid line) and valence (red dashed line) band edges of binary and ternary zb- III-nitrides relative to the valence band edge of zb-GaN. The blue-star symbols indicate the conduction band edge at Γ-valley for indirect-gap alloys. The direct-to-indirect crossover point of zb-Al0.65Ga0.35N is interpolated by zb-Al0.35Ga0.65N and zb-Al0.65Ga0.35N when the conduction band minimum at Γ-valley has the same energy as that of X-valley. The conduction band offsets of zb-GaN/InN, zb-Al0.35Ga0.65N, and zb-Al0.65Ga0.35N are 1.22 and 0.42 eV, which are 0.10 and 0.01 eV smaller than our results obtained using dynamic mixing parameters. The larger deviation of 1.4 ± 0.1 eV measured from inter-sub-band transition energies, where the ratio of the conduction band offset to the band-gap difference is 0.74 ± 0.05. A constant mixing parameter of 0.25 had been reported to study the band gap of zb-AlN and zb-GaN and the band offsets of the zb-AlN/GaN heterojunction. Consequently, the constant mixing parameter of 0.25 significantly underestimates the band gap of zb-AlN and zb-GaN by 0.04 and 0.05 eV, respectively, while the conduction and valence band offsets are 1.22 and 0.42 eV, which are 0.10 and 0.01 eV smaller than our results obtained using dynamic mixing parameters.
explain the relatively small bowing, whereas the cation-like wz-InN. The anion-like conduction band edges in wz-AlGaN mole fraction of Ga and turns into a cation-like character in anion-like behavior; however, it dwindles as the increasing Γ conduction band minimum of wz-AlN at projected electronic structure of wz-AlN, GaN, and InN, the bowing in both wz- and zb- crystals. Revealed by the element-conduction band edge of ternary alloys, except AlGaN, exhibits green colormap indicates an anion-like character, while the light green colormap implies cation-like behavior. From observation in Figures 2 and 3, the valence band edge of ternary alloys can be linearly interpolated, though with a slight upward bowing for AlInN and InGaN. This is because the valence band maximum of AlN, GaN, and InN is composed mainly of anion orbital states regardless of wz- or zb- crystals. The anion-like character makes the valence band edge less sensitive to group-III alloying, which leads to the small bowing of valence band offsets. The slight upward bowing on the valence band edges of AlInN and InGaN can be ascribed to the energy shift of the valence band maximum with respect to the average energy of the top three valence bands at Γ-valley.\(^3\)\(^5\) On the contrary, the conduction band edge of ternary alloys, except AlGaN, exhibits large bowing, which dominantly contributes to the band-gap bowing in both wz- and zb- crystals. Revealed by the element-projected electronic structure of wz-AlN, GaN, and InN, the conduction band minimum of wz-AlN at Γ-valley retains anion-like behavior; however, it dwindles as the increasing mole fraction of Ga and turns into a cation-like character in wz-InN. The anion-like conduction band edges in wz-AlGaN explain the relatively small bowing, whereas the cation-like conduction band edges in wz-AlInN and InGaN account for the large bowing. Likewise, the conduction band minima of zb-AlN, GaN, and InN at Γ-valley have the same anion-to-cation transition. Hence, the large bowing in the conduction band edges of zb-AlInN and InGaN is consistent with that of the wz-counterparts. A small bowing in the conduction band edges of zb-AlGaN is observed for zb-GaN, Al0.25Ga0.75N, and Al0.5Ga0.5N, but not for zb-Al0.75Ga0.25N and AlN because the conduction band minimum of zb-Al0.75Ga0.25N and AlN shifts from Γ-valley to X-valley. In comparison with the anion-like Γ-valley, X-valley has a strong cation-like character. Therefore, the conduction band minimum of zb-Al0.75Ga0.25N and AlN at Γ-valley has the expected small bowing, but the conduction band minimum of zb-Al0.75Ga0.25N and AlN at X-valley behaves oppositely.

By comparing the band offsets of the zb- alloys with those of the wz- alloys, the larger conduction band offset of the zb-GaN/InN heterojunction implies that LEDs made out of zb-GaN/InGaN quantum wells have a better electron capture rate, which suppresses electron leakage current. Likewise, the larger valence band offset of zb-AlN/GaN heterojunctions indicates a better hole capture rate in zb-AlGaN/GaN quantum wells. However, the conduction band offset of zb-AlN/GaN heterojunctions is significantly smaller than that of wz-AlN/GaN heterojunctions because zb-AlN has a smaller indirect band gap of 5.0–5.3 eV. Indeed, if we only consider the Γ-valley where the direct band gap occurs, the conduction band offsets of zb-AlGaN/GaN heterojunctions are identical to those of wz-AlGaN/GaN ones. For instance, the conduction band offsets of the zb-Al0.25Ga0.75N/GaN and zb-AlN/GaN

| heterojunction | \(\Delta E_c\) (eV) | \(\Delta E_{c}^{\exp}\) (eV) | \(\Delta E_v\) (eV) | \(\Delta E_{v}^{\exp}\) (eV) | \(\frac{\Delta E_{c}}{\Delta E_{v}}\) | ref |
|---------------|-----------------|-----------------|-----------------|-----------------|-----------------|------|
| wz-GaN/InN    | 1.60            | 1.65 ± 0.25     | 1.15            | 1.05 ± 0.25     | 0.58            | 31   |
| wz-ALN/GaN    | 2.47            | 2.50 ± 0.10     | 0.30            | 0.30 ± 0.10     | 0.89            | 32   |
| wz-ALN/InN    | 4.07            | 4.10 ± 0.10     | 1.45            | 1.40 ± 0.10     | 0.74            | 33   |
| zb-GaN/InN    | 1.85            | 0.89            | 0.50 ± 0.10     | 0.75            | 34   |
| zb-ALN/GaN    | 1.32            | 1.40 ± 0.10     | 0.43            | 0.50 ± 0.10     | 0.74            | 33   |
| zb-ALN/InN    | 3.17            | 1.32            | 0.71            |                |                 |      |

*The ratios of conduction band offsets to band-gap differences are listed. The experimental conduction band offsets \(\Delta E_{c}^{\exp}\) are derived by assuming that the band gaps of wz-AlN, wz-GaN, wz-InN, zb-ALN, and zb-GaN are 6.2, 3.4, 0.7, 5.3, and 3.3 eV, respectively.

Figure 4. Element-projected electronic structure of (a) wz-AlN, (b) wz-GaN, (c) wz-InN, (d) zb-AlN, (e) zb-GaN, and (f) zb-InN. The red–light green colormap indicates an anion-like character, while the light green–blue colormap represents cation-like behavior.
heterojunctions are 0.57 and 2.51 eV in comparison with those of 0.52 and 2.47 eV in wz-AlN/GaN, respectively. The advantages of zb-AlN/ GaN heterojunctions are determined. An eight-atom simple orthorhombic unit cell, the bulk calculations, the conduction and valence band edges are calculated under the density functional theory (DFT) framework implemented in the Vienna ab initio simulation package (VASP). Projector-augmented wave pseudopotentials with a cutoff kinetic energy of 500 eV are employed. Simulations are boiled down to bulk and slab calculations. In the bulk calculations, the conduction and valence band edges relative to the average electrostatic potential of the unit cell are determined. An eight-atom simple orthorhombic unit cell, which has the lattice vector \( \mathbf{c} \) parallel to (1010), is built for the wz- III-nitrides, while an eight-atom conventional cell is built for the zb- III-nitrides. A 6 × 4 × 4 and 5 × 5 × 5 Γ-centered Monkhorst–Pack set of k-points are sampled for the wz- and zb- unit cells, respectively. Local density approximation (LDA) and generalized gradient approximation (GGA) are well-known approaches to study the exchange–correlation interaction of ground-state electrons, but the excited states and band gap of III–V materials are commonly underestimated, which results in the inaccurate electron affinity and band offset overestimation. Therefore, the HSE06 functional, which fixes band-gap underestimation by mixing the Hartree–Fock exchange energy with the Perdew–Becke–Ernzerhof (PBE) exchange energy, is adopted to describe the exchange–correlation interaction of III-nitrides. The optimal mixing parameters (\( \alpha \)) of 0.341, 0.302, and 0.271 are found to reproduce the experimental band gaps of wz-AlN, GaN, and InN, respectively, while the optimal \( \alpha \) of ternary III-nitrides is linearly interpolated by

\[
\alpha = 0.341 \cdot x + 0.302 \cdot y + 0.271 \cdot (1 - x - y)
\]

where \( x \) and \( y \) are the Al and Ga mole fractions, respectively. Details of finding the optimal \( \alpha \) and accuracy of the linear interpolation are summarized in the supporting information (Figure S1). In the slab calculations, the vacuum energy is extracted using the macroscopic average of the electrostatic potential in the III-nitride thin film as a reference level. However, the thickness of the III-nitride thin film in the slab calculations should be large enough to recover the bulk-like electrostatic potential. According to the convergence tests (Figure S2), a 12-layer III-nitride thin film is large enough to recover the bulk-like electrostatic potential, which guarantees the accuracy of electron affinity. Therefore, 12-layer wz- and zb-slabs terminated with nonpolar (1010) and (110) facets are generated from the converged bulk structures, respectively. An 18 Å vacuum space is reserved in the slabs. A 3 × 2 × 1 and 2 × 2 × 1 Γ-centered Monkhorst–Pack set of k-points is sampled for the wz- and zb-slabs, respectively. Each atom in the slabs is fully relaxed so that the interatomic force and energy difference are smaller than 0.01 eV Å\(^{-1}\) and 10\(^{-6}\) eV, respectively. The macroscopic average of the electrostatic potential along the growth direction \( z \) of slabs is estimated by

\[
\overline{V}(z) = \frac{1}{l_A} \int_{-l_A/2}^{l_A/2} \int dx dy dz \Theta\left(\frac{l}{2} - |z - z'|\right) V(x, y, z')
\]

where \( l, A, \Theta, \) and \( V \) are the interlayer distance along the \( z \)-direction, the cross-sectional area of the slabs perpendicular to the \( z \)-direction, the Heaviside function, and the three-dimensional electrostatic potential of the slabs, respectively. The inner integral averages the electrostatic potential over the periodic directions so-called microscopic average, while the outer integral averages the periodic oscillation of the microscopic potential along the growth direction. Under the assumption that the average electrostatic potential of unit cell is identical to the macroscopic average of the electrostatic potential in the III-nitride thin film of the slabs, the electron affinity can be extracted by

\[
\chi = (E_{\text{vac}} - \overline{V}_{\text{slab}}) - (E_g + \text{VBM} - \overline{V}_{\text{bulk}})
\]

where \( E_{\text{vac}} \) and \( \overline{V}_{\text{slab}} \) are the vacuum energy and the macroscopic average of the electrostatic potential in the III-nitride thin film procured from the slab calculations, while \( E_g \), VBM, and \( \overline{V}_{\text{bulk}} \) are the band gap, the valence band maximum, and the average electrostatic potential of the unit cell obtained from the bulk calculations, respectively.
Figure S1 and Table S1 examine the accuracy of the hybrid density functional theory on the band gap of wzn and zb binary III-nitrides calculated using different Hartree–Fock mixing parameters; and Figure S2 shows the electron affinity of wzn-GaN as a function of thin film thickness (PDF).
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