

Composition-dependent $\mathbf{k} \cdot \mathbf{p}$ band parameters for wurtzite (Al,Ga)N alloys from density functional theory

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Ultraviolet light emitters based on the semiconductor alloy aluminum gallium nitride, (Al,Ga)N, have attracted significant interest in recent years due to their potential for optoelectronic devices. To guide the design of such devices with improved efficiencies, theoretical frameworks based on so-called $\mathbf{k} \cdot \mathbf{p}$ methods have found widespread application in the literature. Given that $\mathbf{k} \cdot \mathbf{p}$ models are empirical in nature, parameters such as effective masses or crystal-field splitting energies of (Al,Ga)N alloys have to be provided as input from first-principles calculations or experiment. Although these parameters are available for GaN and AlN, detailed information on their composition dependence is sparse. Here, we address this question and provide (Al,Ga)N band parameters for widely used multiband $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians. We start from density functional theory (DFT) to sample the electronic structure of (Al,Ga)N alloys over the full composition range. The $\mathbf{k} \cdot \mathbf{p}$ band parameters are treated as free parameters to reproduce the DFT data. For GaN and AlN, the parameters extracted here agree well with literature values. When turning to the composition dependence of the $\mathbf{k} \cdot \mathbf{p}$ parameters, our calculations show that most parameters deviate significantly from a linear interpolation of the GaN and AlN values, an approximation widely made in the literature. Moreover, to describe changes in the band parameters with Al content, *composition-dependent* bowing parameters have to be considered for an accurate description of the DFT data. Finally, our analysis also provides initial insight into consequences of the nonlinear composition dependence of the $\mathbf{k} \cdot \mathbf{p}$ parameters for the electronic structure of (Al,Ga)N alloys. We find that, in particular, the band ordering is affected by the nonlinear evolution of the crystal-field splitting energy with composition, which is an important aspect for the light polarization characteristics of high Al content (Al,Ga)N alloys.

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I. INTRODUCTION

Optoelectronic devices operating in the ultraviolet (UV) spectral region are of interest for a variety of different applications, including biomedicine and disease diagnostics [1–3]. Furthermore, UV sterilization and disinfection [4,5] received strong attention in fighting the coronavirus and its variants [6]. Current UV light emission relies to a large extent on bulky, inefficient, and wavelength non-tunable gas lasers [7] or lamps utilizing toxic mercury [8]. In recent years, the semiconductor alloy aluminum gallium nitride, (Al,Ga)N, has been targeted for replacing these inefficient and environmentally unfriendly devices as the direct (Al,Ga)N band gaps cover, in principle, the

wavelength range from UV-A (315–400 nm) to UV-B (280–315) into the UV-C (200–280 nm) [9].

Although (Al,Ga)N-based UV light emitters present an attractive option for solid-state-based solutions, the efficiency of these devices is currently low, especially in the deep UV (UV-C) spectral range [10,11]. Several aspects contribute to these low efficiencies, including low light extraction efficiencies (LEEs) and *p*-doping of (Al,Ga)N layers with high Al contents [9,10]. In general, the low LEE is tightly linked to fundamental differences in the valence band structure of AlN and GaN systems [12]: The valence band maximum (VBM) in AlN is of Γ_7 symmetry while in GaN it is of Γ_9 symmetry [13,14]. Optical transitions involving the conduction band minimum (CBM) and VBM result in transverse magnetic (TM) polarized light in AlN while in GaN the emitted light is of transverse electric (TE) polarization [15,16]. Given that (Al,Ga)N-based LEDs are mainly top or bottom emitting devices, TM polarized emission contributes to a low LEE [17]. Moreover, in (Al,Ga)N QWs, which form the active region of an LED, several further factors impact the valence-band ordering,

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including strain and quantum confinement but also the magnitude and sign of the so-called crystal-field splitting (CF) energy, Δ_{cf} [12]. For AlN, Δ_{cf} is negative (in the range -164 to -295 meV), while in GaN it is positive and significantly smaller in magnitude (< 40 meV) [18–22]. Understanding how Δ_{cf} changes with alloy content plays an important role in designing (Al,Ga)N-based light emitters, as it will affect the band ordering and thus polarization characteristics of the emitted light. However, as mentioned above, not only is the crystal-field splitting energy important but also quantum-confinement effects will impact the valence-band ordering in (Al,Ga)N heterostructures. Therefore, the effective electron and hole masses of the alloy along, for instance, the growth direction of a quantum well (QW) are key.

Device-level modeling of, for example, (Al,Ga)N-based LEDs largely relies on self-consistent Schrödinger-Poisson solvers that are coupled with drift-diffusion simulations [23,24]. For the wide-band gap system (Al,Ga)N, the Schrödinger equation is widely treated in the framework of $6 + 2$ band $\mathbf{k} \cdot \mathbf{p}$ models [25–27]. Such an approach requires, e.g., effective masses as well as crystal-field splitting energies as input. Parameters for binary AlN and GaN systems have been extracted from experiment but more often from first-principles calculations. However, information on the composition dependence of these parameters in an (Al,Ga)N alloy is sparse. Often, a linear interpolation of the binary parameters with the Al content x is employed to describe an $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloy [28–31]. Nevertheless, several studies have indicated that, for example, the crystal-field splitting energy exhibits deviations from such linear composition behavior [14,32], while others report a linear dependence [33]. Building on this, it is unclear whether a linear interpolation of effective mass parameters is justified.

In this work, we provide information on the composition dependence of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ band parameters. More specifically, we report hole and electron effective mass parameters, which are required for $6 + 2$ band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians that underlie widely available device simulation packages. We determine Luttinger-like $A_i(x)$ with $i = 1, \dots, 6$ parameters and the effective electron mass $m_e(x)$ as a function of the AlN content x over the entire range of composition. In addition, we also study the composition dependence of the crystal-field splitting energy $\Delta_{\text{cf}}(x)$. To do so, we use density functional theory (DFT) to obtain effective electronic band structures of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys, which are then fitted with our $6 + 2$ band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. Our procedure relies on a Sobol sequence that recently has been used to obtain $\mathbf{k} \cdot \mathbf{p}$ parameters for Hamiltonians with larger basis sets, e.g., a 16 band Hamiltonian, from DFT band structures [34]. In general, we follow the procedure established by Rinke *et al.* [22] to extract $\mathbf{k} \cdot \mathbf{p}$ parameters. Our determined $\mathbf{k} \cdot \mathbf{p}$ parameters for AlN and GaN agree well with previously

published values [21,22]. Moreover, our calculations further support that the crystal-field splitting energy deviates noticeably from a linear interpolation of the binary material values. In addition, we find that the effective mass parameters deviate significantly from linearly interpolated values and can be strongly composition dependent. Finally, when using the extracted composition dependent $A_i(x)$ and $\Delta_{\text{cf}}(x)$ parameters for band structure calculations, we observe noticeable deviations in ordering and orbital character of the valence bands when compared with band structures predicted from linearly interpolated $A_i(x)$ and $\Delta_{\text{cf}}(x)$ values. The difference in band ordering can be of strong importance when investigating light polarization characteristics of (Al,Ga)N-based devices. Thus, our extracted parameters present an ideal starting point for device-level simulations to further understand the impact of the material parameters for properties of light-emitting devices.

The manuscript is organized as follows. We first describe the DFT approach underlying our calculations of (Al,Ga)N band structures in Sec. II A. The $\mathbf{k} \cdot \mathbf{p}$ model and the connected fitting procedure are discussed in Sec. II B. In Sec. III, we present the results of our study, namely the composition dependent $m_e(x)$, $A_i(x)$, and $\Delta_{\text{cf}}(x)$ parameters for $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. Moreover, we examine the impact of the obtained parameters on electronic bulk band structures of (Al,Ga)N alloys.

II. THEORY

In this section, we outline the ingredients of the theoretical framework used to extract composition-dependent $\mathbf{k} \cdot \mathbf{p}$ parameters for (Al,Ga)N alloys. We start in Sec. II A with details of the DFT simulations, which form the basis of our $\mathbf{k} \cdot \mathbf{p}$ fitting procedure. In Sec. II B, details of the $\mathbf{k} \cdot \mathbf{p}$ model are given before turning to the fitting approach.

A. Density functional theory calculations

The DFT calculations carried out in this work are based on the plane-wave-based Vienna *Ab Initio* simulation package (VASP) version 5.4.4 [35]. We employ the generalized gradient approximation (GGA), as implemented in the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional, using the projector augmented wave scheme. The semicore d electrons of Ga are treated as valence electrons and the plane wave cutoff energy is 600 eV. The convergence criteria were 1×10^{-4} eV for the energy minimization and 1×10^{-3} eV/Å for the forces in the ionic relaxations. Our DFT calculations have been performed for unstrained bulk systems, thus, we do not consider effects from an underlying substrate. Structural relaxation was achieved by minimizing the pressure on the supercell.

Spin-orbit coupling (SOC) effects require further attention. In GaN, the magnitudes of the crystal-field splitting and the SOC energies are comparable, although both parameters exhibit significant variation across the

literature. Reported SOC values typically lie in the range $\Delta_{\text{so}}^{\text{GaN}} = 17$ meV to $\Delta_{\text{so}}^{\text{GaN}} = 19$ meV, which are much smaller when compared with other III-V materials, e.g., GaAs ($\Delta_{\text{so}}^{\text{GaAs}} = 341$ meV) [20,21]. The crystal splitting energies in GaN span $\Delta_{\text{cf}}^{\text{GaN}} = 9$ meV to $\Delta_{\text{cf}}^{\text{GaN}} = 38$ meV [20–22]; this quantity is absent in zinc blende III-V materials. In contrast, AlN exhibits a pronounced disparity between these quantities: SOC values remain close to $\Delta_{\text{so}}^{\text{AlN}} = 19$ meV, whereas crystal-field splitting energies range between $\Delta_{\text{cf}}^{\text{AlN}} = -164$ meV and $\Delta_{\text{cf}}^{\text{AlN}} = -295$ meV [20–22]. The near-identical SOC energies in GaN and AlN suggest that alloying is unlikely to induce SOC variations of sufficient magnitude to compete with the much stronger crystal-field splitting contribution in AlN. The substantial difference in crystal-field splitting energies between GaN and AlN, including its change in sign, constitutes the primary factor governing valence-band ordering in (Al,Ga)N alloys. This ordering directly determines the optical polarization characteristics [14,15], which are central to the performance of, for example, deep-UV emitters. Thus, we neglect SOC effects as it significantly increases the computational load while introducing only small changes to the band structure, at least in the context of valence-band ordering. This is a widely used approach in DFT calculations for III-N materials [36–40].

The above outlined DFT framework has been chosen for several reasons for our $\mathbf{k} \cdot \mathbf{p}$ parameter extraction. First, even though the PBE-GGA functional underestimates the band gap of GaN and AlN, previous literature studies show that effective *electron* masses obtained from this DFT setup agree well with data extracted from functionals that predict band gaps closer to experiment [41,42]. Second, in comparison to state-of-the-art Heyd, Scuseria, and Ernzerhof (HSE) hybrid functionals [43,44], the PBE-GGA functional is computationally less demanding. Therefore, it allows for a numerically efficient way to screen larger numbers of alloy configurations (see below) and Al contents x to determine $\mathbf{k} \cdot \mathbf{p}$ parameters for $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. Additionally, in case of HSE-DFT, the exact exchange mixing parameter, α , has to be determined and specified. Previous studies have shown that, to obtain a good description of the bulk band gaps of GaN and AlN, the required α values for the two materials, GaN ($\alpha = 0.294$) and AlN ($\alpha = 0.337$), are (very) different [45]. Thus, for an alloy, there is uncertainty on how to determine α . In contrast, in the PBE-GGA functional, there is no free parameter and therefore no further input is required for (Al,Ga)N alloys. Finally, and as we will show below, the valence band effective mass parameters extracted from our PBE-GGA calculations are in good agreement with literature values on GaN and AlN binary materials. Therefore, in terms of effective mass parameters, the PBE-GGA functional should provide a reliable framework over the full composition range in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys.

For the binary GaN and AlN systems, a four atom primitive unit cell with a Γ centered $6 \times 6 \times 4$ k -point

mesh has been used. To treat $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys, we have employed a 72 atom supercell and considered Al contents of $x = 0.11, 0.25, 0.50, 0.75$, and 0.89 . In the supercell case, the Γ centered k -point mesh is $3 \times 3 \times 2$. Starting from experimental findings [46–48], we treat (Al,Ga)N as a random alloy, thus Al and Ga atoms are randomly distributed in the supercell. To account for the impact of the alloy microstructure, for each alloy content x , the electronic structure of 10 random alloy configurations has been investigated.

The discussed DFT framework can now provide electronic band structures for extracting $\mathbf{k} \cdot \mathbf{p}$ parameters. Details of the fitting procedure are given in the following section, where we first introduce the $\mathbf{k} \cdot \mathbf{p}$ model employed.

B. $\mathbf{k} \cdot \mathbf{p}$ model and band structure fitting approach

Following the study by Rinke *et al.* [22], our $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian is expanded in the basis states $|\text{S}\uparrow\rangle$, $|\text{X}\uparrow\rangle$, $|\text{Y}\uparrow\rangle$, $|\text{Z}\uparrow\rangle$, $|\text{S}\downarrow\rangle$, $|\text{X}\downarrow\rangle$, $|\text{Y}\downarrow\rangle$, $|\text{Z}\downarrow\rangle$. The explicit form of the Hamiltonian is given in Appendix A. Although, in general, the chosen basis states lead to a so-called eight-band model, thus accounting for the coupling between s -like conduction and $p_{x,y,z}$ -like valence bands, device simulations of (Al,Ga)N heterostructures often treat valence and conduction bands separately [49–51]. This approximation is, in general, justified by the large band gap of the alloy (> 3.5 eV). Decoupling conduction and valence bands helps to reduce the computational burden when connecting self-consistent Schrödinger-Poisson solvers with drift-diffusion models for device simulations. Bearing this in mind, we consider in the following a $2 + 6$ band $\mathbf{k} \cdot \mathbf{p}$ model. However, it should be noted that the DFT band structures used for $\mathbf{k} \cdot \mathbf{p}$ parameter extraction account intrinsically for conduction and valence band coupling effects. Therefore, even though the fitting is carried out with a $2 + 6$ band $\mathbf{k} \cdot \mathbf{p}$ model, coupling effects are implicitly built into the parameters obtained.

When it comes to fitting $\mathbf{k} \cdot \mathbf{p}$ to DFT band structures, we treat the effective electron mass, m_e , valence band effective mass parameters, A_i with $i = 1, \dots, 6$, and crystal-field splitting energy, Δ_{cf} , as free parameters. Here, it should be noted that in an (Al,Ga)N alloy, disorder will also lead to band mixing effects [52,53]. On the one hand, it is important to capture these effects in the fitting procedure, as this can affect the polarization of the emitted light from (Al,Ga)N systems, and potentially the LEE of a device [53]. On the other hand, no extra terms can be added to the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian discussed above and in Appendix A. This restriction is introduced to ensure that our model parameters are directly applicable to widely available (commercial) software packages, which, in general, only allow defining input parameters for the Hamiltonian but not a “new” Hamiltonian. To account for this constraint, but also to capture alloy disorder-induced band mixing effects and lifting of degeneracies, we proceed as follows. In general,

SOC introduces band mixing effects but also a lifting of degeneracies in bulk $\mathbf{k} \cdot \mathbf{p}$ band structures. Therefore, we use this parameter to mimic the effect of alloy disorder on the band structure of (Al,Ga)N alloys. For example, at $\mathbf{k} = \mathbf{0}$, the energies of the three highest lying valence band states in a semiconductor with a wurtzite crystal structure can be written as follows [54]:

$$E_{\text{VB}_1} = E_v + \Delta_{\text{cf}} + \frac{\Delta_{\text{sp}}}{3}, \quad (1)$$

$$E_{\text{VB}_2} = E_v + \frac{3\Delta_{\text{cf}} - \Delta_{\text{sp}}}{6} + \sqrt{\left(\frac{3\Delta_{\text{cf}} - \Delta_{\text{sp}}}{6}\right)^2 + 2\left(\frac{\Delta_{\text{sp}}}{3}\right)^2}, \quad (2)$$

$$E_{\text{VB}_3} = E_v + \frac{3\Delta_{\text{cf}} - \Delta_{\text{sp}}}{6} - \sqrt{\left(\frac{3\Delta_{\text{cf}} - \Delta_{\text{sp}}}{6}\right)^2 + 2\left(\frac{\Delta_{\text{sp}}}{3}\right)^2}. \quad (3)$$

Compared with Ref. [54], we assumed that $\Delta_{\text{sp}} = \Delta_2 = \Delta_3$, which describes the SOC energy. Moreover, our Δ_{cf} corresponds to Δ_1 in Ref. [54] and is the crystal-field splitting energy. In the absence of SOC and alloy disorder, two of the three valence bands (neglecting spin) are degenerate $E_{\text{VB}_1} = E_{\text{VB}_2} \neq E_{\text{VB}_3}$. In this case, the band ordering depends on the sign of Δ_{cf} . For our purpose, Δ_{sp} and Δ_{cf} are introduced as free parameters to account for alloy-disorder-induced valence-band splitting effects in (Al,Ga)N alloys, especially at the Γ -point. Thus, in conjunction with DFT data on the energetic separation of the highest lying three valence bands at the Γ -point, Eqs. (1)–(3) are used to obtain an initial guess for Δ_{sp} and Δ_{cf} when targeting data away from the Γ -point.

It is important to note that the SOC term is just an effective means to capture disorder-induced valence-band splittings, especially at the Γ -point, without altering the Hamiltonian structure and allowing for disorder-induced band-mixing effects. Intrinsically, we still assume an ideal C_{6v} symmetry, the standard assumption in $\mathbf{k} \cdot \mathbf{p}$ modeling of (Al,Ga)N systems. In general, alloy disorder will break the C_{6v} symmetry and as a result, additional matrix elements may, in principle, arise, which can further modify the band ordering, orbital character, and optical selection rules, including spin splittings [55]. The magnitude of such terms depends on the specific perturbation. However, the broad success of $\mathbf{k} \cdot \mathbf{p}$ models in optoelectronic device simulations suggests that this simplified description captures the dominant physics to first order.

Certainly, there is scope for more advanced treatments. This includes introducing new and additional $\mathbf{k} \cdot \mathbf{p}$ parameters in the Hamiltonian itself or by advanced fitting strategies. These advanced strategies may go beyond

fitting of energies and effective masses, and could incorporate the orbital character of the valence bands, which can be extracted from DFT output.

Overall, our approach advances multiband $\mathbf{k} \cdot \mathbf{p}$ modeling for (Al,Ga)N by replacing the weakly justified linear interpolation of the $\mathbf{k} \cdot \mathbf{p}$ parameters with a DFT-motivated interpolation scheme that captures the alloy-dependent valence-band dispersion. It provides a consistent implementation of the widely used assumption that symmetry-breaking effects, such as disorder-induced off-diagonal Hamiltonian terms, can be neglected to first order, with their influence effectively absorbed into the alloy-dependent $\mathbf{k} \cdot \mathbf{p}$ parameters. Since band ordering and mixing in heterostructures depend not only on alloy composition but also on quantum-confinement effects at well-barrier interfaces, our resulting parameter set will offer an advanced basis for modeling (Al,Ga)N heterostructures and deep-UV devices, while remaining fully compatible with existing (commercial) simulation frameworks.

In terms of the numerical routine used to fit $\mathbf{k} \cdot \mathbf{p}$ to DFT band structures and thus to extract the $\mathbf{k} \cdot \mathbf{p}$ parameters outlined above, we follow Marquardt *et al.* [34]. Here, we use a Monte Carlo fitting scheme [56] based on a Sobol sequence method [57,58]. Sobol sequences have been shown to yield superior results as compared with several other low-discrepancy point fitting techniques and as a natural substitute to usual random sequences; further details on the employed approach can be found in Refs. [34,59]. The $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian and the Monte Carlo fitting scheme are implemented in the flexible, generalized multiband $\mathbf{k} \cdot \mathbf{p}$ formalism within the plane-wave framework of the SPHInX library [59–61].

When it comes to selecting DFT data for $\mathbf{k} \cdot \mathbf{p}$ fitting, we follow largely the work by Rinke *et al.* [22]. Thus, for our $\mathbf{k} \cdot \mathbf{p}$ parameter extraction, we chose the directions Σ , Λ , T , and Δ in the first Brillouin zone. More specifically, we fit (a) $\Gamma \rightarrow \frac{M}{20}$ (Σ path), (b) $\Gamma \rightarrow \frac{L}{20}$ (Λ path), (c) $\Gamma \rightarrow \frac{K}{20}$ (T path), and (d) $\Gamma \rightarrow \frac{A}{10}$ (Δ path) simultaneously. Given the underlying assumptions of the $\mathbf{k} \cdot \mathbf{p}$ method used here, i.e., a perturbation theoretical approach at the Γ -point, our fitting procedure focuses on the region close to the Γ -point. For the $\mathbf{k} \cdot \mathbf{p}$ parameter extraction, equal path lengths have been covered. Furthermore, a high density of DFT k -points has been chosen along the different directions for accurate parameter extraction (≥ 30 points). To determine the $\mathbf{k} \cdot \mathbf{p}$ parameters for AlN and GaN, the parameter sets of Vurgaftman and Meyer [21] have been used as an initial guess. To reduce the likelihood that the fitting procedure converges to a local minimum, the $\mathbf{k} \cdot \mathbf{p}$ parameters are allowed to be varied by plus and minus the magnitude of the respective initial guess value. We have tested the impact of both changing initial guess values as well as the range over which the parameters are allowed to be varied on the resulting final parameter set. In general, both factors (initial guess and parameter range) had a negligible impact

on the final $\mathbf{k} \cdot \mathbf{p}$ parameter set. For (Al,Ga)N alloys, we generally employ the same procedure, except that the initial guess for our alloy $\mathbf{k} \cdot \mathbf{p}$ parameters is obtained as a linear interpolation of our GaN and AlN values. Each of the ten random alloy configurations considered per alloy content is fitted individually along the four high-symmetry paths. The final $\mathbf{k} \cdot \mathbf{p}$ parameters are obtained by averaging over these ten fits.

III. RESULTS

In this section, we present (i) results of the above outlined parameter extraction procedure and (ii) consequences of the obtained composition-dependent $\mathbf{k} \cdot \mathbf{p}$ parameters for the valence band structure of (Al,Ga)N alloys. In Sec. III A, we summarize our $\mathbf{k} \cdot \mathbf{p}$ parameters for GaN and AlN systems and compare the obtained data with available literature values. The $\mathbf{k} \cdot \mathbf{p}$ parameters extracted for (Al,Ga)N alloys are discussed in Sec. III B. Finally, in Sec. III C, we compare electronic band structures of (Al,Ga)N alloys calculated using our composition-dependent $\mathbf{k} \cdot \mathbf{p}$ parameters with band structures obtained when employing a linear interpolation of the values for GaN and AlN found in Sec. III A.

A. GaN and AlN parameters

Figure 1 displays the DFT band structure together with the fitted $\mathbf{k} \cdot \mathbf{p}$ band structure for two of the four considered directions in the first Brillouin zone for (a) GaN and (b) AlN. To quantify the quality of the $\mathbf{k} \cdot \mathbf{p}$ fit, we use the root mean square deviation (RMSD) and the normalized RMSD [62,63]. Across both materials, the RMSD values indicate very good agreement between the $\mathbf{k} \cdot \mathbf{p}$ and target DFT band structures. For AlN, the valence band normalized RMSDs remain below 3.1% of the fitted energy window, with absolute deviations around 0.1 meV, and the CBM fit is similarly good (0.1 meV, 0.17%). GaN shows slightly larger but still small deviations, with valence band RMSDs of 1.3%–4.8% and absolute errors of 0.1–2.6 meV; the CBM is also very well reproduced (0.54 meV, 0.56%). We attribute the larger deviation in the GaN case to the band anticrossing region in the valence band along the $\Gamma \rightarrow K/20$ path, cf. Fig. 1. To capture this particular aspect of the band structure in detail, additional terms in the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian, such as the A_7 -parameter and/or SOC, need to be considered. In our case, given that the DFT calculations are performed in the absence of SOC, the splitting can be attributed to the A_7 term when using a $\mathbf{k} \cdot \mathbf{p}$ based analysis. In general, the A_7 -term is linear in k [22] and often neglected or explicitly set to zero in $\mathbf{k} \cdot \mathbf{p}$ models for nitride-based heterostructures [30,51,64,65]. This is often motivated by the observation that in III-V materials it presents a small correction and does not affect the VBM very close to the Γ -point. Including the A_7 parameter in the here used $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian would yield an even closer match to the

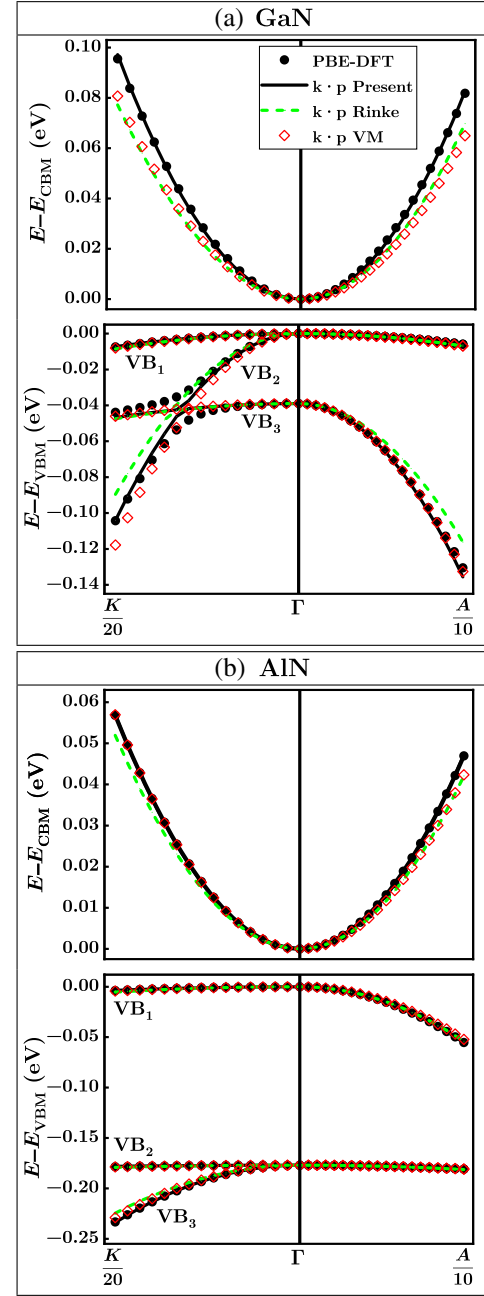


FIG. 1. Band structure of wurtzite (a) GaN and (b) AlN in the vicinity of the Γ -point. Our PBE-DFT data are presented by filled black circles and the fitted $\mathbf{k} \cdot \mathbf{p}$ band structures by the solid black line. Band structures using the $\mathbf{k} \cdot \mathbf{p}$ parameter sets from Rinke *et al.* [22] and Vurgaftman and Meyer (VM) [21] are given by dashed green lines and red open diamonds, respectively. To focus on differences in the dispersion, the band structures are plotted with respect to the conduction and valence band edges, respectively. Moreover, the crystal-field splitting energy of our PBE-DFT calculations is used for all $\mathbf{k} \cdot \mathbf{p}$ calculations.

PBE-DFT band structures. However, we can see also from Fig. 1 that for AlN the band anticrossing region would not be encountered in the k -point range considered in the fitting procedure. This will make it difficult to constrain the A_7

TABLE I. Band parameters for AlN, GaN, and (Al,Ga)N alloys when accounting for bowing parameters b , α , and β . Definitions of these parameters are given in the main text and Appendix C. Effective electron mass values parallel and perpendicular to the c axis have been denoted by superscripts $\parallel$ and $\perp$, respectively. Literature values from Rinke *et al.* [22] and Vurgaftman and Meyer [21] are given for comparison. Percentage differences between values obtained in the present study and literature data are given in brackets. Three center dots (...) indicate that data is not available, has not been calculated; see main text for discussion.

Band parameters	Materials						b	α	β
	GaN			AlN					
	Present	Ref. [22]	Ref. [21]	Present	Ref. [22]	Ref. [21]			
A_1	-7.438	-5.947 (20.0%)	-7.21 (3.1%)	-4.101	-3.991 (2.7%)	-3.86 (5.9%)	...	-5.48	3.46
A_2	-0.485	-0.528 (8.9%)	-0.44 (9.3%)	-0.211	-0.311 (47.4%)	-0.25 (18.5%)	...	-1.07	6.35
A_3	6.965	5.414 (22.3%)	6.68 (4.1%)	3.822	3.671 (4.0%)	3.58 (6.3%)	...	5.46	5.00
A_4	-2.963	-2.512 (15.2%)	-3.46 (16.8%)	-1.487	-1.147 (22.9%)	-1.32 (11.2%)	...	-0.29	-0.89
A_5	-2.998	-2.510 (16.3%)	-3.40 (13.4%)	-1.632	-1.329 (18.6%)	-1.47 (9.9%)	...	-2.40	0.33
A_6	-4.352	-3.202 (26.4%)	-4.90 (12.6%)	-2.11	-1.952 (7.5%)	-1.64 (22.3%)	...	-3.84	0.88
Δ_{cf} (eV)	0.040	0.034 (15.0%)	0.010 (75.0%)	-0.177	-0.295 (66.7%)	-0.169 (4.52%)	...	-0.19 (eV)	-0.22
Δ_{sp} (eV)	...	...	...	...	...	...	...	-0.07 (eV)	-0.91
$m_e^\perp(m_0)$	0.166	0.209 (25.9%)	0.20 (20.0%)	0.300	0.329 (9.7%)	0.30 (0.0%)	-0.060	2.38	1.06
$m_e^\parallel(m_0)$	0.150	0.186 (24.0%)	0.20 (33.3%)	0.287	0.322 (12.2%)	0.32 (11.5%)	-0.052	3.80	0.85

value for AlN. For this reason and following the widely made approximation in the literature, we do not account for the A_7 parameter in the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. Moreover, and as we will see below for the alloy case, where we include a SOC-like coupling parameter, the anticrossing region of the band structures can be captured well even without including an A_7 -term in the Hamiltonian. In general, our analysis reveals a very good agreement between the $\mathbf{k} \cdot \mathbf{p}$ and the DFT band structure, highlighting that both GaN and AlN are accurately described by our $\mathbf{k} \cdot \mathbf{p}$ model in the chosen $\mathbf{k}$ range. The extracted valence band $\mathbf{k} \cdot \mathbf{p}$ parameters A_i , electron effective mass values parallel, $m_e^\parallel$, and perpendicular, $m_e^\perp$, to the c axis, as well as the crystal-field splitting energy Δ_{cf} are summarized in Table I.

To compare our data with existing literature data, Fig. 1 also displays $\mathbf{k} \cdot \mathbf{p}$ band structures when using the A_i and m_e parameter sets from Vurgaftman and Meyer [21] as well as Rinke *et al.* [22]. To focus on the band dispersion, the band structures are always plotted with respect to CBM and VBM. Moreover, the crystal-field splitting energies from our calculations have been used for all parameter sets. Our DFT calculations give $\Delta_{cf}^{\text{AlN}} = -177$ meV for AlN and $\Delta_{cf}^{\text{GaN}} = 40$ meV for GaN. The obtained AlN value is in good agreement with that reported by Vurgaftman and Meyer [21] ($\Delta_{cf}^{\text{AlN,VM}} = -169$ meV) but it is noticeably smaller in magnitude than the value reported by Rinke *et al.* ($\Delta_{cf}^{\text{AlN,Rinke}} = -295$ meV) [22]. However, for GaN, our data on the crystal splitting energy agree well with the value reported by Rinke *et al.* ($\Delta_{cf}^{\text{GaN,Rinke}} = 34$ meV) [22]. Vurgaftman and Meyer [21] suggest a smaller value ($\Delta_{cf}^{\text{GaN,VM}} = 10$ meV). In general, one should note that the work in Ref. [21] is a summary and average of parameters reported in the literature.

Looking at the energy dispersion of AlN, Fig. 1(b), we find that over the $\mathbf{k}$ -point range considered, all three parameter sets give band structures in very good agreement with each other, in particular for the valence band structure. The different $\mathbf{k} \cdot \mathbf{p}$ parameter sets are summarized and compared in Table I. For GaN, Fig. 1(a), we observe some deviations between the three $\mathbf{k} \cdot \mathbf{p}$ parameter sets; however, very close to the Γ -point the band structures do not differ significantly; differences near the valence band anticrossing region are related to nonvanishing A_7 parameters in Refs. [21,22]. The comparison with Refs. [21,22] in Table I shows that our extracted electron effective masses are slightly lower than previously reported values. To probe the origin of these differences, we performed additional DFT calculations using the modified Becke-Johnson (mBJ) functional, which reproduces HSE-DFT band gaps at far lower computational cost [66]. However, the mBJ calculations yielded higher electron masses (not shown) than both our PBE-DFT results and the literature values in Refs. [21,22], indicating that the functional alone does not explain the discrepancy. Since effective masses depend on the energy and k -point range used in the fitting procedure, we also examined the impact of extending the fitted band structure region. Increasing the k -range to match that used by Rinke *et al.* [22] leads to larger extracted masses and brings our results into even closer agreement with Ref. [22], as shown in Table II. These tests confirm that the PBE functional yields effective masses consistent with the literature. At the same time, the underlying assumptions of the $\mathbf{k} \cdot \mathbf{p}$ approach, namely its perturbative validity only in the immediate vicinity of the Γ -point, imply that shorter path lengths are the more appropriate choice for this semiempirical method. Given the general good agreement between our

TABLE II. GaN and AlN electron effective mass values parallel and perpendicular to the c axis for the path length used for the fitting procedure. Literature values from Rinke *et al.* [22] are given for comparison. Path length, L_1 , is the path length used for all calculations in this work. Path length two, L_2 , is the path length considered in Ref. [22]. Percentage differences between values obtained in the present study and literature data are given in brackets.

	GaN		Ref. [22]
	L_1	L_2	
$m_e^\perp(m_0)$	0.166 (25.9%)	0.192 (8.9%)	0.209
$m_e^\parallel(m_0)$	0.150 (24.0%)	0.175 (6.3%)	0.186

	AlN		Ref. [22]
	L_1	L_2	
$m_e^\perp(m_0)$	0.30 (9.7%)	0.314 (4.8%)	0.329
$m_e^\parallel(m_0)$	0.287 (12.2%)	0.303 (6.27%)	0.322

data and the literature values for GaN and AlN, in the next section we extract $\mathbf{k} \cdot \mathbf{p}$ parameters for (Al,Ga)N alloys.

B. (Al,Ga)N alloy parameter

In this section, we focus on the composition dependence of the $\mathbf{k} \cdot \mathbf{p}$ parameters of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. We start by investigating the effective electron mass, both $m_e^\perp(x)$ and $m_e^\parallel(x)$, of (Al,Ga)N alloys. Subsequently, we study the valence band effective mass parameters $A_i(x)$. As discussed above, we use ten different random alloy configurations per Al content x in the considered $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys and fit each individual band structure with the $\mathbf{k} \cdot \mathbf{p}$ model. The final parameter set is then obtained as an average over the ten different configurations. Figure 2 displays an example of our $\mathbf{k} \cdot \mathbf{p}$ fit to an effective $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ DFT band structure (arbitrarily selected alloy configuration). Further examples of the $\mathbf{k} \cdot \mathbf{p}$ fits to the PBE-DFT data for all alloy compositions and the four considered paths are provided in Appendix D. As Fig. 2 shows, the $\mathbf{k} \cdot \mathbf{p}$ band structure is in very good agreement with the DFT data over the $\mathbf{k}$ -point range considered. This highlights that (i) the $\mathbf{k} \cdot \mathbf{p}$ model is suitable for describing the alloy band structure and (ii) that the SOC-like term in our $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian captures the alloy-induced lifting of degeneracies in the band structure well. We note that alloy disorder breaks the translational symmetry of the crystal, which results in the situation that Bloch's theorem is in principle no longer applicable. Thus, defining a band structure is not strictly valid. However, $\mathbf{k} \cdot \mathbf{p}$ descriptions of alloys assume that perturbations of disorder are weak and that an effective band structure can still be assumed. To bridge the gap between disorder and effective band structures, we have constructed supercells

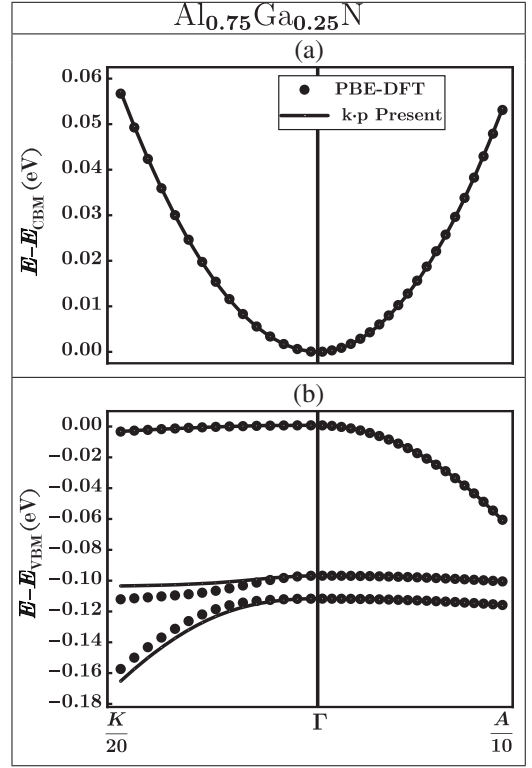


FIG. 2. (a) Conduction and (b) valence band structure of an $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ random alloy in the vicinity of the Γ -point. Our PBE-DFT data are presented by filled black circles and the fitted $\mathbf{k} \cdot \mathbf{p}$ band structures by the solid black line.

that are large enough to capture disorder effects on an atomistic level but small enough so that electrons with low $\mathbf{k}$ -vectors move in the periodic potential due to the periodic boundary conditions of the plane-wave DFT approach used. In doing so, effects of alloy disorder are included in a limit that is consistent with the underlying assumptions of a $\mathbf{k} \cdot \mathbf{p}$ model.

1. Effective electron masses

To gain insight into the composition dependence of the effective electron mass in (AlGa)N alloys, we follow here previous literature and distinguish between effective electron masses perpendicular, $m_e^\perp(x)$, and parallel, $m_e^\parallel(x)$, to the c axis. The effective electron masses are extracted according to the above outlined fitting procedure considering the in-plane directions Σ , Λ , T , and the out-of-plane direction Δ in the first Brillouin zone. The obtained masses are displayed in Fig. 3 as a function of the Al content x in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. In Fig. 3(a), the mass $m_e^\perp$ perpendicular to the c axis is shown while (b) displays the mass $m_e^\parallel$ parallel to the c axis. To evaluate the impact of alloy content x on the effective electron mass, Fig. 3 also shows the effective mass values for the two directions obtained by a linear interpolation of the effective mass values of GaN and AlN via:

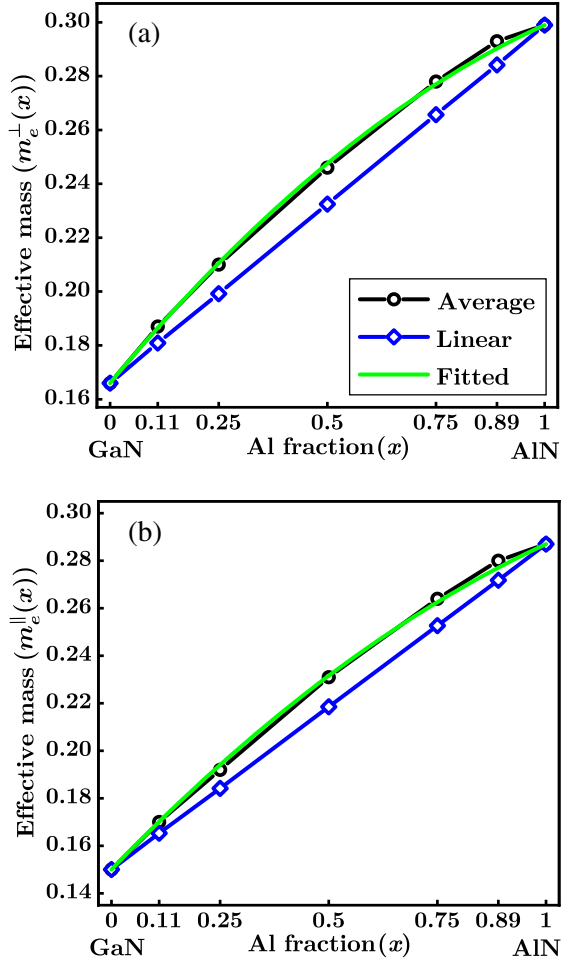


FIG. 3. Conduction band effective masses of (Al,Ga)N alloys for (a) perpendicular, $m_e^\perp$, and (b) parallel, $m_e^\parallel$, to the wurtzite c axis.

$$m_{e,\text{AlGa}N}^\alpha = x m_{e,\text{AlN}}^\alpha + (1-x) m_{e,\text{Ga}N}^\alpha, \quad (4)$$

where $\alpha = \{\perp, \parallel\}$ denotes the directions. The corresponding data are given in Fig. 3 by the blue line (open blue diamonds). We note that different approaches have been used in the literature to estimate the effective electron mass of an alloy [67–69]. To compare our results with recent literature data by Balestra *et al.* [41], we use Eq. (4) as their DFT data indicate a Vegard law-type behavior for the composition dependence of the effective electron masses in (Al,Ga)N. However, in Appendix C, we discuss an alternative, widely used approach. From Fig. 3 we infer that both for $m_e^\perp$ and $m_e^\parallel$ our data deviate from a linear interpolation of the effective electron masses via Eq. (4). It should be noted that our extracted electron masses do not differ significantly when extracted from the ten different microscopic configurations at each Al content x (the largest deviation is 1.65% from the average value). The differences between our results and Ref. [41] may be due to several factors. Although in general the approach used

in Ref. [41] is similar to ours, which means that it also utilizes PBE-DFT, the region over which the band structure is fitted to extract the effective electron masses may be different. Furthermore, the supercell employed in Ref. [41] is smaller (32-atoms) when compared with ours (72 atoms). Further studies would be required to elucidate the differences between our work and Ref. [41].

To provide an improved description of the composition dependence of the effective electron masses but also to extrapolate to composition values not explicitly studied here, we adapt the widely used expression for the band gap evolution [70,71] of semiconductor alloys to effective electron masses and introduce a bowing parameter:

$$m_{e,\text{AlGa}N}^\alpha = x m_{e,\text{AlN}}^\alpha + (1-x) m_{e,\text{Ga}N}^\alpha - b(1-x)x. \quad (5)$$

Figure 3 reveals that $m_e^\perp(x)$ and $m_e^\parallel(x)$ are indeed well described by Eq. (5), thus when introducing the bowing parameter b . The effective electron mass bowing parameters obtained are summarized in Table I.

2. Valence band $\mathbf{k} \cdot \mathbf{p}$ parameters

Having discussed the composition dependence of the electron effective mass in (Al,Ga)N alloys, we turn now and focus on the composition dependence of the valence band effective mass parameters A_i with $i = 1, \dots, 6$, crystal-field splitting energy, Δ_{cf} , and the alloy disorder parameter, Δ_{sp} . We start the analysis with the parameters $A_i(x)$, which are shown in Fig. 4 as a function of the Al content x in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. The black open circles give the average values of $A_i(x)$, including error bars, from the fitting to PBE-DFT band structures. Again, to visualize the impact of alloy disorder on $A_i(x)$, Fig. 4 also shows $A_i(x)$ parameters obtained (blue open diamonds) when employing the often used linear interpolation (Vegard's law) of the GaN and AlN parameters with composition x [28–31]. Except for $A_4(x)$, the data obtained from a linear interpolation noticeably deviate from the PBE-DFT values.

Moreover, when trying to describe the composition dependence of the $A_i(x)$ parameters similar to the effective electron mass values via a composition-independent bowing parameter:

$$A_i^{\text{AlGa}N} = x A_i^{\text{AlN}} + (1-x) A_i^{\text{Ga}N} - b_i^{\text{A}_i}(1-x)x, \quad (6)$$

the PBE-DFT is poorly approximated. An example for such a poor fitting to the PBE-DFT data via Eq. (6) is given in Fig. 5 for $A_1(x)$ as an example. A similar behavior is observed for the other $A_i(x)$ parameters (not shown here). In general, this finding suggests that the bowing parameter itself is composition *dependent*. A similar behavior has been observed for the band gap bowing in (In,Ga)N [72,73] but in particular in (Al,In)N alloys [74–76]. In the case of the band gap bowing of (Al,In)N, Sakalauskas *et al.* [74] introduced an empirical formula to account for

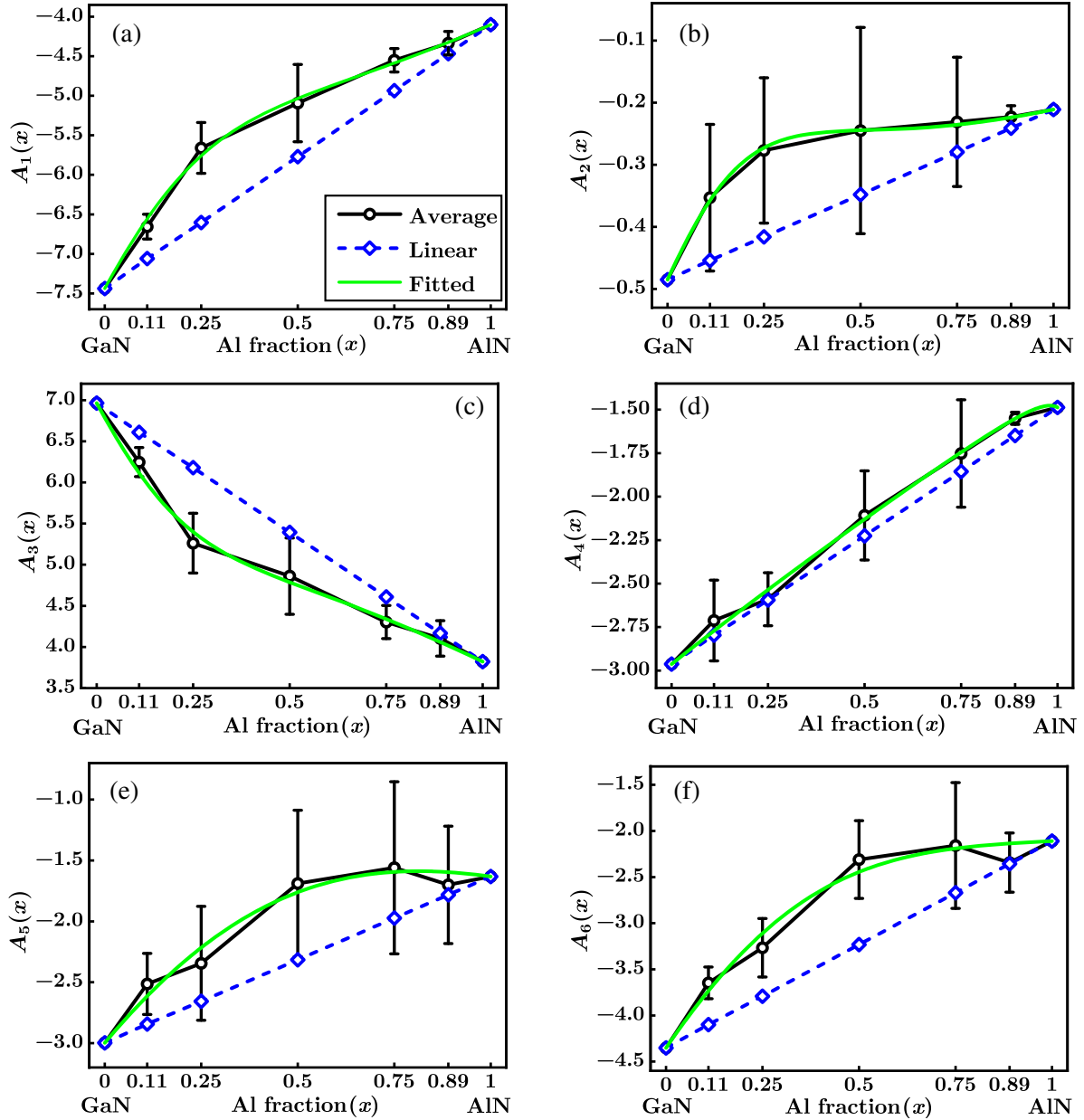


FIG. 4. Luttinger-like parameter $A_i(x)$ with $i = 1, \dots, 6$ (from (a) to (f) in the figure) as a function of the alloy content x of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. The black circles represent the average value of A_i parameters over ten random alloy configurations per x ; the blue diamonds denote the values obtained from a linear interpolation of the AlN and GaN A_i values. The solid green lines are obtained using Eq. (7); see main text for further details.

the composition dependence of the bowing parameter. We have adopted this approach here for the valence effective mass parameters $A_i(x)$:

$$\begin{aligned} A_i^{\text{AlGa}} &= xA_i^{\text{AlN}} + (1-x)A_i^{\text{Ga}} - \frac{\alpha_i}{1 + \beta_i x^2}(1-x)x \\ &= xA_i^{\text{AlN}} + (1-x)A_i^{\text{Ga}} - \tilde{b}_i^{A_i}(x)(1-x)x. \end{aligned} \quad (7)$$

Here, α_i and β_i are free parameters which are used to fit the averaged PBE-DFT data for each $A_i(x)$. Figure 4

shows indeed that Eq. (7) allows to capture the composition dependence of the A_i parameters over the full composition range. Moreover, Eq. (7) enables us also to predict A_i parameters at compositions not explicitly targeted in the PBE-DFT calculations. The obtained α_i and β_i values for the different A_i parameters are summarized in Table I.

Having presented the results for the effective mass parameters $A_i(x)$, we turn in a second step to the composition dependence of the crystal-field splitting energy, Δ_{cf} , and the alloy disorder parameter, Δ_{sp} .

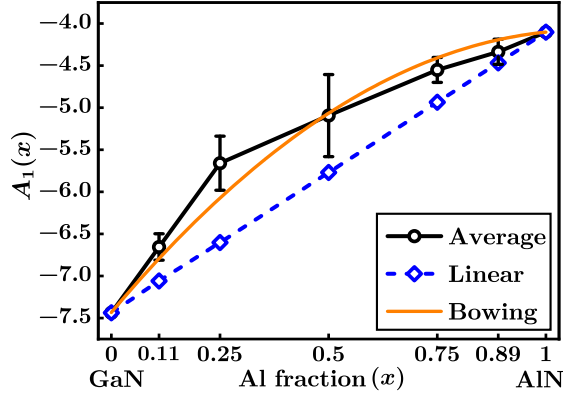


FIG. 5. Luttinger-like parameter $A_1(x)$ as a function of the Al content x of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. The black circles represent the average value of A_1 over ten random alloy configurations per x while the blue diamonds denote the values obtained from a linear interpolation of the AlN and GaN A_1 values. The solid orange line is obtained by fitting the data with a composition-independent bowing parameter, Eq. (6). See main text for further details.

Figure 6(a) shows $\Delta_{\text{cf}}(x)$ as a function of the Al content x in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ while Fig. 6(b) depicts the data for $\Delta_{\text{sp}}(x)$. Looking at Fig. 6(a), one observes that the $\Delta_{\text{cf}}(x)$ values extracted from PBE-DFT (black open circles) noticeably deviate from a linear interpolation (blue open diamonds) of the GaN and AlN crystal-field splitting values. The evolution of Δ_{cf} with x is again well described by a *composition-dependent* bowing parameter of the form $\tilde{b}_{\text{cf}}(x) = \alpha_{\text{cf}}/(1 + \beta_{\text{cf}}x^2)$, as used for the A_i parameters in Eq. (7). The extracted values α_{cf} and β_{cf} are given in Table I. As discussed above, the sign of Δ_{cf} plays an important role for the polarization characteristics of light emitted from (Al,Ga)N alloys. Assuming that carriers only occupy the highest valence band and in the absence of band mixing effects, a positive (negative) crystal-field splitting energy $\Delta_{\text{cf}}(x)$ suggests TE (TM) polarized light emission. Given the nonlinear behavior of $\Delta_{\text{cf}}(x)$ with composition x , Fig. 6(a) indicates that the onset of a polarization switching from TE to TM occurs at higher Al contents x when compared with a linear interpolation of $\Delta_{\text{cf}}(x)$ with composition x . The dashed lines show the critical Al content x_{cr} at which the sign of Δ_{cf} changes. In case of a linear interpolation of Δ_{cf} , $x_{\text{cr}}^{\text{lin}} \approx 0.18$. When accounting for the composition-dependent bowing parameter $\tilde{b}_{\text{cf}}(x)$ for predicting $\Delta_{\text{cf}}(x)$, $x_{\text{cr}}^{\text{bow}} \approx 0.41$.

The evolution of Δ_{cf} with composition has been targeted in the literature before. Some studies come to the conclusion that $\Delta_{\text{cf}}(x)$ deviates from the linear interpolation of the binary values of GaN and AlN [14,32], while others predict a close to linear behavior [33]. However, a direct comparison with existing literature data is difficult. First, experimental studies providing information on the polarization switching are usually carried out on samples that are strained to a substrate. One can in principle account for

strain effects when estimating the crossover for the unstrained case, although it requires information on (i) the valence band deformation potentials and their composition dependence and (ii) crystal-field splitting energies of the binary materials. As already discussed in Sec. III A, in the literature there is a large spread in AlN and GaN values for Δ_{cf} and the valence and conduction band deformation potentials [77,78]. The closest to our study here are the empirical tight-binding model (ETBM) calculations by Coughlan *et al.* [14], which predict that Δ_{cf} changes sign at $x_{\text{cr}}^{\text{ETBM}} = 0.25$. However, the calculations in Ref. [14] use different binary Δ_{cf} values for GaN, $\Delta_{\text{cf}}^{\text{GaN, ETBM}} = 23$ meV, and AlN, $\Delta_{\text{cf}}^{\text{AlN, ETBM}} = -240$ meV, when compared with the values obtained here from PBE-DFT calculations ($\Delta_{\text{cf}}^{\text{GaN}} = 40$ meV and $\Delta_{\text{cf}}^{\text{AlN}} = -177$ meV). Using our composition-dependent bowing parameter formula with $\Delta_{\text{cf}}^{\text{GaN}} = 23$ meV and $\Delta_{\text{cf}}^{\text{AlN}} = -240$ meV from Ref. [14], we obtain that Δ_{cf} changes sign at $x_{\text{cr}} = 0.20$, which is close to the value obtained by Coughlan *et al.* [14]. Thus, the composition-dependent bowing parameter obtained here reflects well the ETBM results in Ref. [14] when accounting for differences in the crystal-field splitting energies. In general, further studies focusing on detailed theory-experiment comparisons, especially in terms of the optical transitions [33], are required to fully explore and analyze the evolution of Δ_{cf} with alloy content x in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers.

As already mentioned above, the sign of the crystal-field splitting energy gives a first indication for changes in the valence band structure. However, alloy disorder also leads to band mixing effects and a lifting of degeneracies. We mimicked this effect through an SOC-like interaction term, introducing a single free parameter, Δ_{sp} , in the Hamiltonian. In doing so, the developed method is compatible with $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians underlying widely available (commercial) software packages. Figure 6(b) displays Δ_{sp} as a function of the Al content x . The data are again fitted with a bowing parameter of the form $\tilde{b}_{\text{sp}}(x) = \alpha_{\text{sp}}/(1 + \beta_{\text{sp}}x^2)$; α_{sp} and β_{sp} values for Δ_{sp} are summarized in Table I. As there is no alloy disorder in GaN and AlN, for the binary systems $\Delta_{\text{sp}} = 0$ meV. Overall, we observe that Δ_{sp} can be of similar magnitude to Δ_{cf} in the Al content composition range up to 50%–60%. For higher Al contents $\Delta_{\text{sp}} < |\Delta_{\text{cf}}|$. We also observe that Δ_{sp} is largest between $x = 0.75$ and $x = 0.89$, thus indicating that alloy disorder impacts the electronic structure in the high AlN content regime more strongly. A similar observation has been made by Finn and Schulz when studying the electronic structure of (Al,Ga)N QWs by means of an atomistic ETBM [52].

C. Impact of composition-dependent $\mathbf{k} \cdot \mathbf{p}$ parameter on (Al,Ga)N band structures

As discussed above, Δ_{cf} and Δ_{sp} will impact both valence-band ordering and mixing, which will affect the light polarization characteristics of (Al,Ga)N alloys. In the

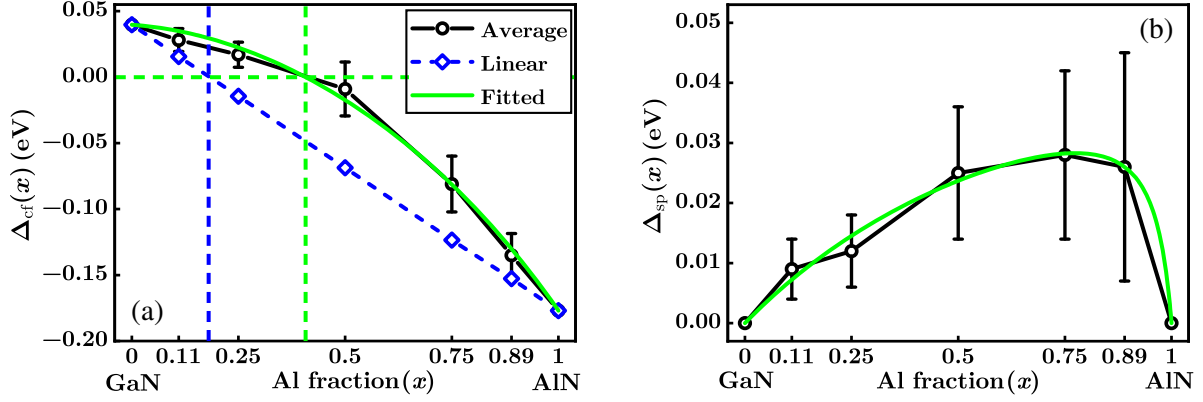


FIG. 6. Composition dependence of (a) crystal-field splitting energy $\Delta_{cf}(x)$ and (b) the alloy disorder parameter $\Delta_{sp}(x)$ in (Al,Ga)N alloys. Color coding and line styles follow the conventions of Fig. 4.

following, we compare $\mathbf{k} \cdot \mathbf{p}$ band structures of (Al,Ga)N alloys where the underlying parameters are determined by using (i) the composition-dependent bowing parameters, $\tilde{b}$, obtained in the present work and (ii) when linearly interpolating the AlN and GaN parameters and thus also neglecting alloy disorder-induced band mixing effects. Our aim is a general study of changes in the band structure rather than providing detailed insight into light polarization characteristics as this requires accounting for carrier densities and temperature effects, e.g., via a Fermi-Dirac distribution of carriers in the different valence bands. However, we can provide initial information on how the $\mathbf{k} \cdot \mathbf{p}$ parameters can affect the light polarization characteristics of (Al,Ga)N alloys by studying not only the energy dispersion of the different valence bands but also by resolving the orbital character of the different bands as a function of $\mathbf{k}$. For this analysis, we have selected two alloy compositions, namely $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ and $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}$.

In a first step, we study the $\mathbf{k} \cdot \mathbf{p}$ band structure of an $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ alloy. For this Al content, $\Delta_{cf} < 0$ when using a linear interpolation of the GaN and AlN values, as shown in Fig. 6(a). However, when accounting for the composition-dependent bowing parameter, $\tilde{b}(x)$, $\Delta_{cf} > 0$. As mentioned above, the sign of Δ_{cf} gives first insight into the valence-band ordering but does not provide information about band mixing effects or energetic separation of the different valence bands due to disorder. Figure 7(a) shows the band structure of an $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ alloy in the vicinity of the Γ -point for a linear interpolation of the $\mathbf{k} \cdot \mathbf{p}$ parameters with composition, while Fig. 7(b) depicts the band structure when accounting for composition-dependent bowing parameters, $\tilde{b}(x)$. The color coding of the bands gives the orbital character. We have grouped p_x and p_y -like orbital contributions together as they both facilitate TE polarized light emission in contrast to p_z -like states, which generally contribute to TM polarization. Looking at the band structure obtained from the linearly interpolated $\mathbf{k} \cdot \mathbf{p}$ parameters, Fig. 7(a), one finds that the

topmost valence band, denoted as VB_1 in the following, is entirely p_z -like in character. The lower-lying valence states, denoted as VB_2 and VB_3 , are p_x and p_y -like in character. The valence bands VB_2 and VB_3 are degenerate here since neither alloy disorder-related nor small SOC effects are considered in the linearly interpolated $\mathbf{k} \cdot \mathbf{p}$ parameter set. Overall, the band ordering seen in Fig. 7(a) is consistent with a negative Δ_{cf} value [cf. Fig. 6(a)], which means that the topmost valence band is expected to be p_z -like in character. However, even though VB_1 is p_z -like in character and thus suggests TM polarized light emission, VB_2 and VB_3 are only approximately 20 meV below VB_1 . Given that the thermal energy at room temperature ($T = 300$ K) is around 24 meV, one can expect some occupation of VB_2 and VB_3 with holes at this temperature. This in turn will impact the degree of optical polarization, ρ , which can be defined as the ratio of intensities of TE to TM polarized light emission, $\rho = (I_{\text{TE}} - I_{\text{TM}})/(I_{\text{TE}} + I_{\text{TM}})$ [14,79,80] and potentially the LEE in a device. However, in general, the band structure depicted in Fig. 7(a) is indicative of predominantly TM polarized light emission in an $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ alloy when using a linear interpolation of the $\mathbf{k} \cdot \mathbf{p}$ parameters with Al content.

When accounting for the extracted composition-dependent bowing parameters, Fig. 7(b) reveals that the resulting $\mathbf{k} \cdot \mathbf{p}$ valence band structure noticeably deviates from the band structure obtained within the linear interpolation scheme, cf. Fig. 7(a). First, the topmost valence band, VB_1 , is mainly $p_x + p_y$ -like in character at the Γ -point when accounting for composition-dependent bowing parameters. Also VB_2 is predominantly of $p_x + p_y$ -like character near Γ . The degeneracy of VB_1 and VB_2 is lifted due to alloy disorder, here introduced by the Δ_{sp} term in the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. The energetically lowest valence band, VB_3 , is of p_z -like character. It should be noted that VB_3 lies more than 30 meV below the valence band edge. Therefore, thermal occupation of this band at room temperature is

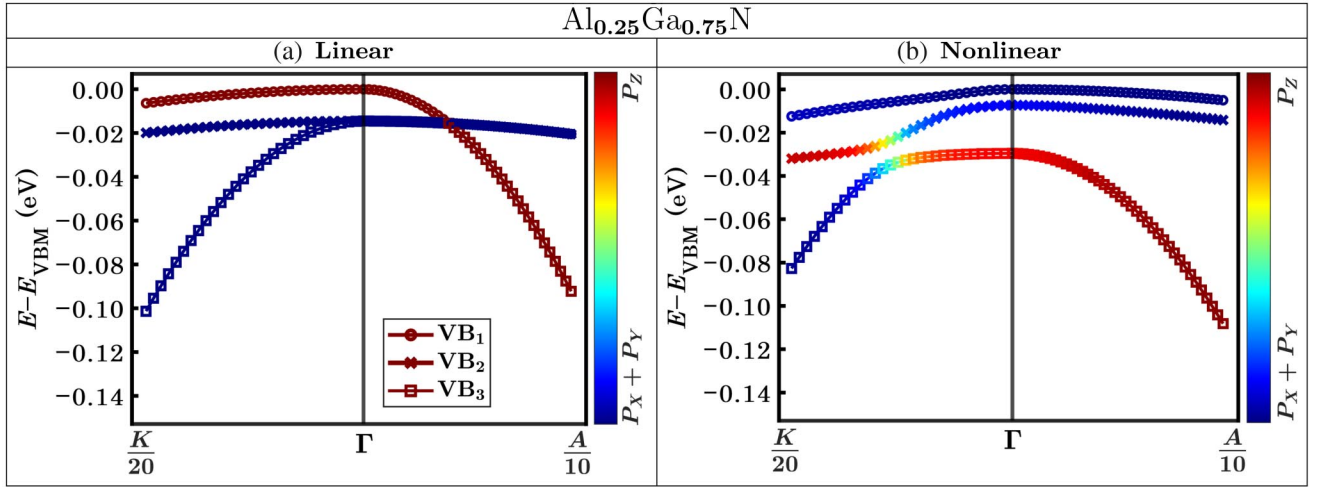


FIG. 7. Band structure of an $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ alloy obtained from (a) linearly interpolated $\mathbf{k} \cdot \mathbf{p}$ parameters and (b) when accounting for alloy disorder effects, Δ_{sp} , and composition-dependent bowing parameters, $\tilde{b}(x)$.

unlikely, at least at low carrier densities. Even though there is some band mixing between VB_2 and VB_3 along the $\Gamma \rightarrow K$ direction away from Γ , predominantly TE polarized light emission is expected when accounting for the composition-dependent bowing parameters, even at elevated temperatures and low carrier densities.

We note again that our discussion is based on unstrained bulk systems. Strain or quantum confinement in, e.g., QWs can lead to further changes in the band structure and band ordering as discussed in the literature [53,81,82]. The effective masses of the different bands play an important role in understanding the impact of quantum confinement on, for instance, the valence-band ordering in a QW system and thus the optical properties. In general, UV light emitters that utilize (Al,Ga)N alloys are grown along the wurtzite c axis [83–85]. Therefore, the effective masses associated with the different valence bands toward the A-point (along the wurtzite c axis) are important and we can now gain information on how these masses depend on the interpolation of the $\mathbf{k} \cdot \mathbf{p}$ parameters. For the calculated band structure, we employed both the analytic expressions provided in Appendix B and numerical differentiation of the band dispersion in the vicinity of the Γ -point to extract the effective masses. Both approaches yield consistent results. Figure 7(a) reveals a low effective hole mass ($m_{\text{VB}_1} = 0.15 m_0$) in this direction for the highest valence band, VB_1 , when using linearly interpolated parameters for the band structure calculation. The energetically lower-lying bands, VB_2 and VB_3 , exhibit much higher effective masses ($m_{\text{VB}_2} = 2.35 m_0$; $m_{\text{VB}_3} = 2.35 m_0$). This suggests that quantum-confinement effects will significantly impact the valence-band ordering, as the topmost valence, VB_1 , will shift to lower energies more strongly when compared with VB_2 and VB_3 . Given the differences in the orbital character of the different valence bands, strong

band mixing effects may be expected in a c -plane $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ QW depending on, e.g., the well width. This will also affect the degree of optical polarization and potentially the LEE. However, when accounting for nonlinearities in the $\mathbf{k} \cdot \mathbf{p}$ parameter interpolation, the situation is different, as Fig. 7(b) shows. In this case, VB_1 and VB_2 exhibit heavier effective masses ($m_{\text{VB}_1} = 2.78 m_0$, $m_{\text{VB}_2} = 1.04 m_0$) toward the A-point, while VB_3 has a low effective mass ($m_{\text{VB}_3} = 0.19 m_0$) in this direction. This means that quantum confinement along the wurtzite c axis will shift VB_3 away from the valence band edge formed by VB_1 and VB_2 . Given that VB_1 and VB_2 are predominantly p_x and p_y -like in orbital character, the energetically highest valence states in an $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ QW will be formed by such orbitals, indicating mainly TE polarized light emission. This reveals a very different result compared with the conclusions drawn from the linearly interpolated $\mathbf{k} \cdot \mathbf{p}$ parameter set presented in Fig. 7(a).

In a second step, we turn our attention to the band structure of $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}$ alloys, which often form the active region or the cladding layer of UV light emitters in the 250–300 nm wavelength range [86–89]. Figure 8(a) shows the band structure resulting from a linear interpolation of the $\mathbf{k} \cdot \mathbf{p}$ parameters with Al content $x = 0.5$. The band structure is largely identical to the band structure displayed in Fig. 7(a) for the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ case: The energetically highest valence band, VB_1 , is of p_z -like character, while the energetically lower-lying valence bands, VB_2 and VB_3 , are $p_x + p_y$ -like in character and degenerate at the Γ -point. The main difference compared with the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ case is that the energetic separation between VB_1 and $\text{VB}_{2,3}$ is much greater at the Γ -point. In the $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}$ alloy, the energetic separation is > 60 meV, compared with only 20 meV for $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$. This behavior is expected when looking at the linear interpolation

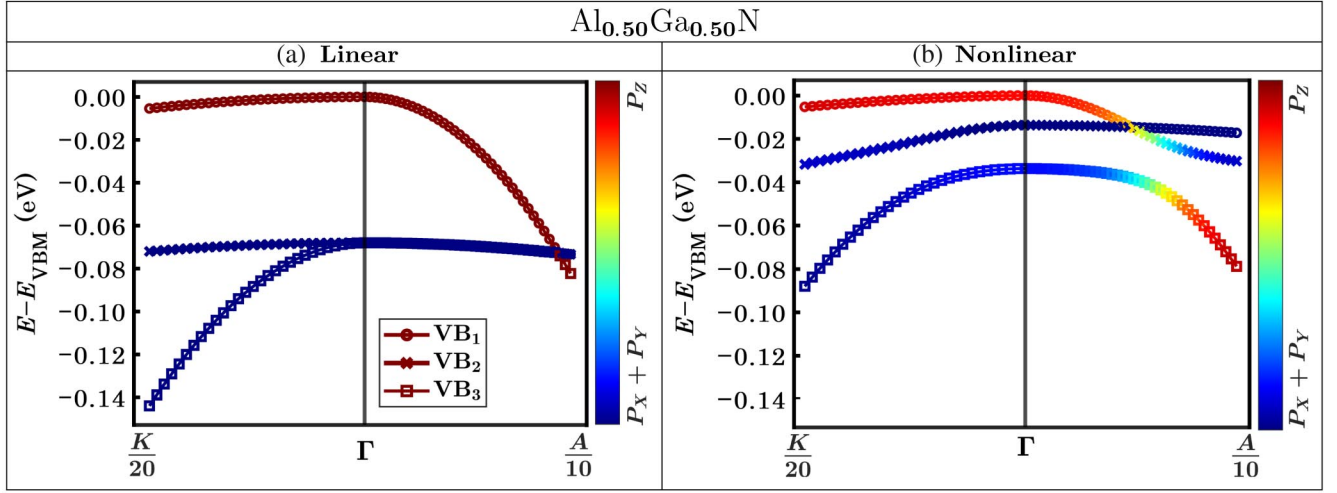


FIG. 8. Band structure of an $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}$ alloy obtained from (a) linearly interpolated $\mathbf{k} \cdot \mathbf{p}$ parameters and (b) when accounting for alloy disorder effects, Δ_{sp} , and composition-dependent bowing parameters, $\tilde{b}(x)$.

of the crystal-field splitting energy with composition [cf. Fig. 6(a)]. As a consequence and in contrast to $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$, thermal occupation of VB_2 and VB_3 is unlikely in the bulk case. Thus, the light emitted from a bulk $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}$ alloy is expected to be TM polarized, at least when using linearly interpolated $\mathbf{k} \cdot \mathbf{p}$ parameters. Turning to the effective masses of the different valence bands toward the A-point, we observe a situation similar to $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$, Fig. 7(a), in the sense that VB_1 ($m_{\text{VB}_1} = 0.17 m_0$) exhibits a low effective mass while VB_2 and VB_3 ($m_{\text{VB}_2} = 2.66 m_0$, $m_{\text{VB}_3} = 2.66 m_0$) have a high effective mass along this direction. Thus, quantum confinement in c -plane $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}$ QWs can reduce the energetic separation between p_z and $p_x + p_y$ -like valence bands. However, given the large crystal-field splitting energy, even in a strong carrier confinement regime, e.g., narrow wells, and when focusing on energetic shifts in the band structure resulting from the different effective masses of the valence bands only (no strain contributions), TM polarized emission may still be expected in the case of the linearly interpolated $\mathbf{k} \cdot \mathbf{p}$ parameters. Strain effects may change this behavior and would have to be further analyzed.

The situation is again different when accounting for composition-dependent bowing parameters in determining the $\mathbf{k} \cdot \mathbf{p}$ parameters of the $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}$ alloy, as the band structure in Fig. 8(b) clearly shows. Although the energetically highest valence band, VB_1 , also has a larger p_z orbital character (87%) near the Γ -point, the energy separation to VB_2 is much smaller (approximately equal to 20 meV) when compared with the band structure obtained from a linearly interpolated set of $\mathbf{k} \cdot \mathbf{p}$ parameters; see Fig. 8(a). Thus, at room temperature, occupation of VB_2 with holes can be expected. Moreover, the orbital character of VB_2 is mainly $p_x + p_y$ -like. Therefore, in the case of a nonlinear interpolation of the $\mathbf{k} \cdot \mathbf{p}$ parameters,

the degree of optical polarization will be determined by the orbital character in the valence bands VB_1 and VB_2 . Looking at the effective masses of the different valence bands near the Γ -point and along the direction of the A-point, we find that VB_1 ($m_{\text{VB}_1} = 0.23 m_0$) has a low effective mass, while VB_2 and VB_3 ($m_{\text{VB}_2} = 4.03 m_0$, $m_{\text{VB}_3} = 1.14 m_0$) exhibit high effective masses. However, given the smaller crystal-field splitting energy in the case of a nonlinear interpolation of the $\mathbf{k} \cdot \mathbf{p}$ parameters, quantum confinement in a c -plane $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}$ QW may now give rise to strong band mixing effects as VB_1 , VB_2 , and VB_3 may be energetically very close and QW states are then formed from all three bands as linear combinations. As such, the degree of optical polarization may be strongly impacted by this effect and may differ from the results predicted when linearly interpolated parameters are used to calculate the QW electronic structure.

IV. CONCLUSION

In summary, we have investigated the composition dependence of $\mathbf{k} \cdot \mathbf{p}$ parameters for wurtzite (Al,Ga)N alloys. These parameters are key ingredients for widely available theoretical and simulation models to analyze electronic, optical, and carrier transport properties of (Al,Ga)N-based heterostructures and devices.

To gain insight into the composition dependence of the $\mathbf{k} \cdot \mathbf{p}$ band parameters, we use PBE-DFT calculations to sample the electronic structure of (Al,Ga)N alloys over the full composition range. The DFT data were fitted with a $\mathbf{k} \cdot \mathbf{p}$ model widely used in the literature. Thus, the obtained $\mathbf{k} \cdot \mathbf{p}$ parameter set is compatible with, for instance, commercially available software packages, which, in general, do not allow users to define “arbitrary” $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians.

Our investigations show that the extracted band parameters for GaN and AlN agree well with literature data. However, our study also reveals that the widely used approximation of a linear interpolation of the GaN and AlN parameter sets with composition breaks down in (Al,Ga)N alloys. To describe the DFT data accurately, composition-dependent bowing parameters are required for most of the (Al,Ga)N $\mathbf{k} \cdot \mathbf{p}$ parameters. We provide here an empirical expression to predict (Al,Ga)N $\mathbf{k} \cdot \mathbf{p}$ band parameters at desired alloy compositions.

Moreover, we furnish initial insight into the consequences of the nonlinear behavior of the $\mathbf{k} \cdot \mathbf{p}$ parameters with Al content for the bulk band structure of (Al,Ga)N alloys. We observed, for example, that band ordering and energetic separation of the different valence bands are strongly impacted by the nonlinear evolution of the $\mathbf{k} \cdot \mathbf{p}$ parameter set with composition. The obtained results indicate that optical properties in (Al,Ga)N bulk alloys but also QW systems can differ significantly depending on whether a linear or nonlinear interpolation scheme to determine the $\mathbf{k} \cdot \mathbf{p}$ parameters is used.

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DATA AVAILABILITY

The data that support the findings of this article are openly available at Ref. [90].

APPENDIX A

The $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian used in the present work is based on the work of Gershoni *et al.* [91] and is also described in Refs. [54,64]. For a wurtzite structure, the 8×8 Hamiltonian in the basis ($|S\uparrow\rangle$, $|X\uparrow\rangle$, $|Y\uparrow\rangle$, $|Z\uparrow\rangle$, $|S\downarrow\rangle$, $|X\downarrow\rangle$, $|Y\downarrow\rangle$, $|Z\downarrow\rangle$) is described in matrix form as

$$\hat{H} = \begin{bmatrix} G(\mathbf{k}) & \Gamma \\ -\Gamma^* & G^*(\mathbf{k}) \end{bmatrix}. \quad (\text{A1})$$

Here, $G(\mathbf{k})$ and Γ are 4×4 matrices and $G(\mathbf{k})$ can be further decomposed into 4×4 matrices:

$$G(\mathbf{k}) = G_1(\mathbf{k}) + G_2(\mathbf{k}) + G_{\text{sp}} + G_{\text{cf}}. \quad (\text{A2})$$

The matrix $G_1(\mathbf{k})$ is given by

$$G_1(\mathbf{k}) = \begin{bmatrix} E_c & iP_2k_x & iP_2k_y & iP_1k_z \\ -iP_2k_x & E_v & 0 & 0 \\ -iP_2k_y & 0 & E_v & 0 \\ -iP_1k_z & 0 & 0 & E_v \end{bmatrix}, \quad (\text{A3})$$

where E_c and E_v are the conduction and valence band edges, respectively. $G_2(\mathbf{k})$ has the following form:

$$G_2(\mathbf{k}) = \begin{bmatrix} A'_2(k_x^2 + k_y^2) + A'_1k_z^2 & B_2k_yk_z & B_2k_xk_z & B_1k_xk_y \\ B_2k_yk_z & L'_1k_x^2 + M'_1k_y^2 + M_2k_z^2 & N'_1k_xk_y & N'_2k_xk_z - N'_3k_x \\ B_2k_xk_z & N'_1k_xk_y & M_1k_x^2 + L'_1k_y^2 + M_2k_z^2 & N'_2k_yk_z - N'_3k_y \\ B_1k_xk_y & N'_2k_xk_z + N'_3k_y & N'_2k_yk_z + N'_3k_y & M_3k_x^2 + M_3k_y^2 + L'_2k_z^2 \end{bmatrix}, \quad (\text{A4})$$

where terms L'_i , N'_i , and M_i are associated with the Luttinger-like parameters A_i with $i = 1, \dots, 6$, while the terms A'_1 and A'_2 are determined by conduction band effective masses $m_e^\perp$ and $m_e^\parallel$, respectively:

$$A'_1 = \frac{\hbar^2}{2m_e^\perp}, \quad A'_2 = \frac{\hbar^2}{2m_e^\parallel}, \quad (\text{A5a})$$

$$L'_1 = \frac{\hbar^2}{2m_0}(A_2 + A_4 + A_5), \quad L'_2 = \frac{\hbar^2}{2m_0}(A_1), \quad (\text{A5b})$$

$$M_1 = \frac{\hbar^2}{2m_0}(A_2 + A_4 - A_5), \quad M_2 = \frac{\hbar^2}{2m_0}(A_1 + A_3), \quad (\text{A5c})$$

$$N'_1 = \frac{\hbar^2}{2m_0}(2A_5), \quad N'_2 = \frac{\hbar^2}{2m_0}(\sqrt{2}A_6), \quad N'_3 = i(\sqrt{2}A_7). \quad (\text{A5d})$$

Following Gershoni *et al.* [91], we set the B parameter to zero. This is consistent with the work of Rinke *et al.* [22], where it is discussed that including this term did not

improve the fitting of the band structures. Moreover, the A_7 parameter is set to zero in our calculations, which is a widely used approximation and makes the model compatible with, e.g., $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians underlying commercially available software packages such as nextnano [92] and Crosslight APSYS [93]. Furthermore, the parameters $P_{1/2}$ that describe conduction band valence band coupling are set to zero, which is also a widely used approximation for wide-band gap materials such as (Al,Ga)N alloys [25,26,94]. The reduced form of the Hamiltonian is often referred to as a 6 + 2 band model.

In the standard definition of the Hamiltonian, Eq. (A1), the matrices G_{sp} and Γ describe the spin-orbit coupling. As discussed in the main text, we use these terms here to account for alloy disorder-induced band mixing and lifting of degeneracies in the band structure of (Al,Ga)N alloys. In general, we use the standard definitions of G_{sp} and Γ in our fitting procedure:

$$G_{\text{sp}} = \frac{\Delta_{\text{sp}}}{3} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (\text{A6})$$

and

$$\Gamma = \frac{\Delta_{\text{sp}}}{3} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -i \\ 0 & -1 & i & 0 \end{pmatrix}. \quad (\text{A7})$$

Finally, the crystal-field splitting contribution, present in the wurtzite crystal structure, is described by

$$G_{\text{cf}} = \Delta_{\text{cf}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{A8})$$

APPENDIX B

Expressions for the effective hole masses parallel and perpendicular to the wurtzite c axis have been given in Refs. [22,54] in terms of the Luttinger-like parameters A_i with $i = 1, \dots, 6$. Following Refs. [22,54] the masses can be calculated close to or far from the Γ -point, and the corresponding equations are summarized below.

1. Hole masses close to Γ -point

$$m_0/m_{\text{VB}_1}^{\parallel} = -(A_1 + A_3), \quad m_0/m_{\text{VB}_1}^{\perp} = -(A_2 + A_4), \quad (\text{B1a})$$

$$m_0/m_{\text{VB}_2}^{\parallel} = -\left[A_1 + \left(\frac{E_{\text{VB}_2}}{E_{\text{VB}_2} - E_{\text{VB}_3}}\right)A_3\right],$$

$$m_0/m_{\text{VB}_2}^{\perp} = -\left[A_2 + \left(\frac{E_{\text{VB}_2}}{E_{\text{VB}_2} - E_{\text{VB}_3}}\right)A_4\right], \quad (\text{B1b})$$

$$m_0/m_{\text{VB}_3}^{\parallel} = -\left[A_1 + \left(\frac{E_{\text{VB}_3}}{E_{\text{VB}_3} - E_{\text{VB}_2}}\right)A_3\right],$$

$$m_0/m_{\text{VB}_3}^{\perp} = -\left[A_2 + \left(\frac{E_{\text{VB}_3}}{E_{\text{VB}_3} - E_{\text{VB}_2}}\right)A_4\right]. \quad (\text{B1c})$$

Here, E_{VB_2} and E_{VB_3} are the energies of the two valence bands at the Γ -point described by Eqs. (2) and (3) in Sec. III B.

2. Hole masses far from Γ -point

$$m_0/m_{\text{VB}_1}^{\parallel} = -(A_1 + A_3), \quad m_0/m_{\text{VB}_1}^{\perp} = -(A_2 + A_4 - A_5), \quad (\text{B2a})$$

$$m_0/m_{\text{VB}_2}^{\parallel} = -(A_1 + A_3), \quad m_0/m_{\text{VB}_2}^{\perp} = -(A_2 + A_4 + A_5), \quad (\text{B2b})$$

$$m_0/m_{\text{VB}_3}^{\parallel} = -A_1, \quad m_0/m_{\text{VB}_3}^{\perp} = -A_2. \quad (\text{B2c})$$

APPENDIX C

Effective masses for semiconductor alloys A_xB_{1-x} are often determined via the harmonic mean [69,95,96]:

$$\frac{1}{m_{e,AB}} = \frac{x}{m_{e,A}} + \frac{1-x}{m_{e,B}}. \quad (\text{C1})$$

To provide bowing parameters for the effective mass parallel and perpendicular to the wurtzite c axis in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys when using the harmonic mean, we follow the general procedure outlined in the main text:

$$\frac{1}{m_{e,\text{AlGa}}^{\lambda}} = \frac{x}{m_{e,\text{AlN}}^{\lambda}} + \frac{1-x}{m_{e,\text{Ga}}^{\lambda}} - \frac{\alpha_{\lambda}}{1 + \beta_{\lambda}x^2}(1-x)x, \quad (\text{C2})$$

where $\lambda \in \{\perp, \parallel\}$. The resulting effective mass data are shown in Fig. 9. The linear interpolation is obtained by setting $\alpha = \beta = 0$. We can see that the reciprocal effective masses, $1/m_{e,\text{AlGa}}^{\lambda}$ differ noticeably from the linear interpolation. The bowing parameters obtained here are $\alpha_{\perp} = 2.38$; $\beta_{\perp} = 1.06$ and $\alpha_{\parallel} = 3.80$; $\beta_{\parallel} = 0.85$.

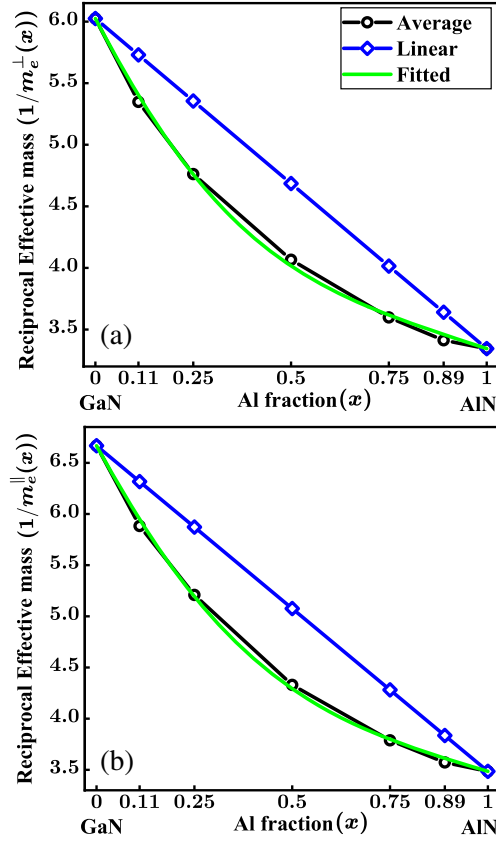


FIG. 9. Reciprocal conduction band effective masses of $(\text{Al,Ga})\text{N}$ alloys for (a) perpendicular, $1/m_e^\perp$, and (b) parallel, $1/m_e^\parallel$, to the wurtzite c axis.

APPENDIX D

In this appendix, we present additional examples of $\mathbf{k} \cdot \mathbf{p}$ band-structure fits to the PBE-DFT data. For each alloy composition, one representative fit is shown along the four paths defined in Sec. II B. Figures 10(a) and 10(b) display the results for $\text{Al}_{0.11}\text{Ga}_{0.89}\text{N}$, while Figs. 10(c) and 10(d) show the corresponding data for $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$. Figure 11 depicts the

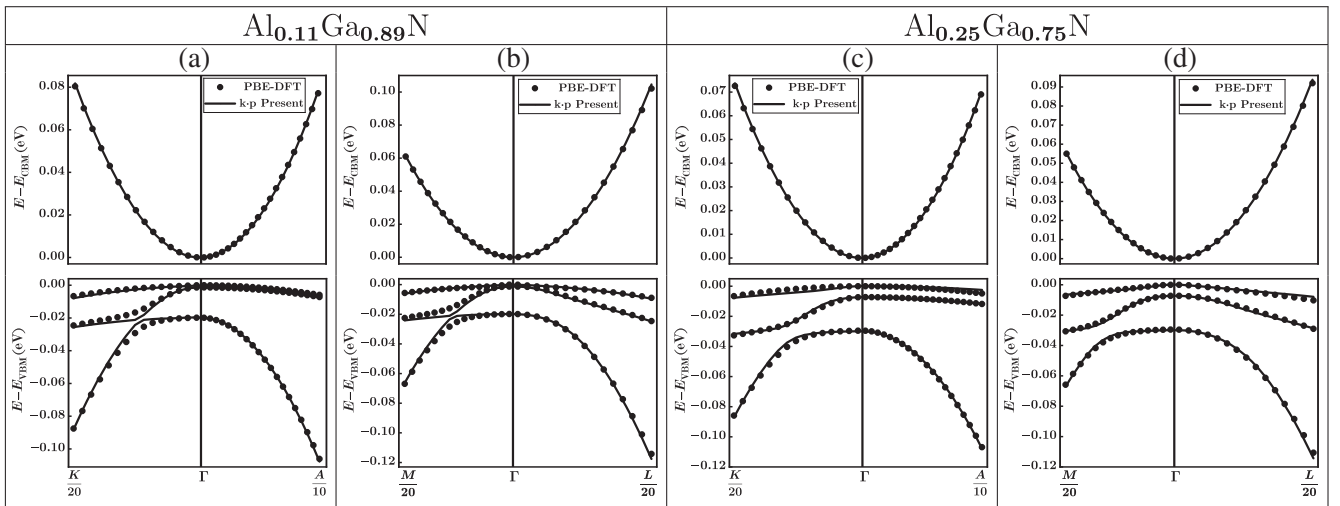


FIG. 10. Conduction and valence band structure of an $\text{Al}_{0.11}\text{Ga}_{0.89}\text{N}$ random alloy in the vicinity of the Γ -point (a) from $K/20 \rightarrow \Gamma \rightarrow A/20$ and (b) along the $M/20 \rightarrow \Gamma \rightarrow L/20$ path; (c),(d) show the band structure along the respective paths for $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$. Our PBE-DFT data are presented by filled black circles and the fitted $\mathbf{k} \cdot \mathbf{p}$ band structures by the solid black line.

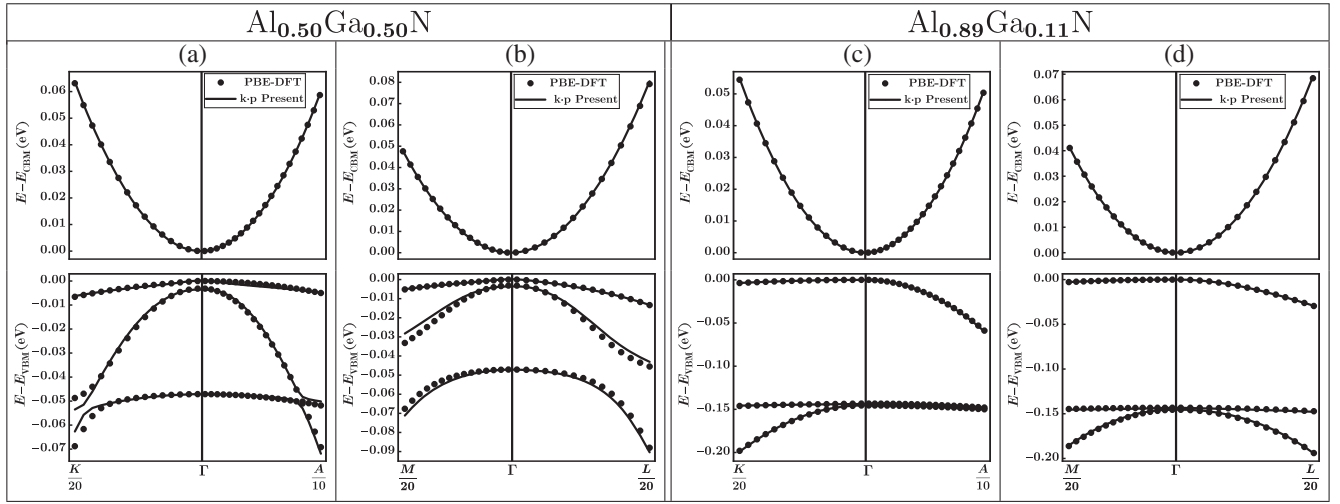


FIG. 11. Conduction and valence band structure of an $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}$ random alloy in the vicinity of the Γ -point (a) from $K/20 \rightarrow \Gamma \rightarrow A/20$ and (b) along the $M/20 \rightarrow \Gamma \rightarrow L/20$ path; (c), (d) show the band structure along the respective paths for $\text{Al}_{0.89}\text{Ga}_{0.11}\text{N}$. Our PBE-DFT data are presented by filled black circles and the fitted $\mathbf{k} \cdot \mathbf{p}$ band structures by the solid black line.

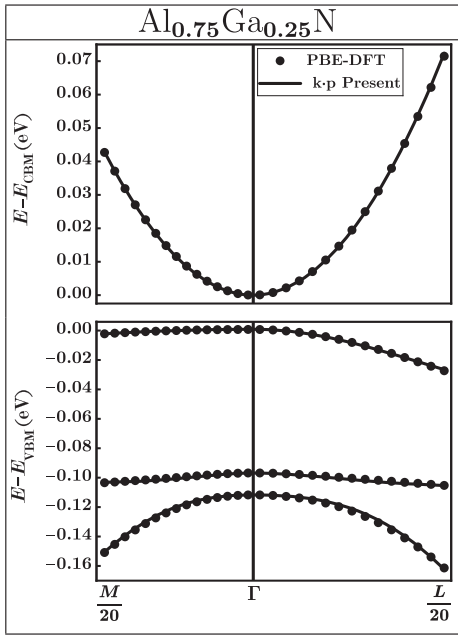


FIG. 12. Conduction and valence band structure of an $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ random alloy in the vicinity of the Γ -point from $M/20 \rightarrow \Gamma \rightarrow L/20$. The data along $K/20 \rightarrow \Gamma \rightarrow A/20$ are shown in the main text. Our PBE-DFT data are presented by filled black circles and the fitted $\mathbf{k} \cdot \mathbf{p}$ band structures by the solid black line.

fits for $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}$ and $\text{Al}_{0.89}\text{Ga}_{0.11}\text{N}$. For $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$, only the $M/20 \rightarrow \Gamma \rightarrow L/20$ path is included here, Fig. 12, as the $K/20 \rightarrow \Gamma \rightarrow A/20$ path is already given in Fig. 2 of the main text.

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