Shielding electrostatic fields in polar semiconductor nanostructures

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Modern opto-electronic devices are based on semiconductor heterostructures employing the process of electron-hole pair annihilation. In particular polar materials enable a variety of classic and even quantum light sources, whose on-going optimisation endeavours challenge generations of researchers. However, the key challenge - the inherent electric crystal polarisation of such materials - remains unsolved and deteriorates the electron-hole pair annihilation rate. Here, our approach introduces a sequence of reverse interfaces to compensate these polarisation effects, while the polar, natural crystal growth direction is maintained provoking a boost in device performance. Former research approaches like growth on less-polar crystal planes or even the stabilization of unnatural phases never reached industrial maturity. In contrast, our solution allows the adaptation of all established industrial processes, while the polarisation becomes adjustable; even across zero. Hence, our approach marks the onset of an entire class of ultra-fast and efficient devices based on any polar material.

Semiconductor structures with thicknesses of a few nanometres are commonly used to confine electrons and holes in close vicinity, which increases the electron-hole pair annihilation rate governing the photon generation. As a result, any dense semiconductor band structure is transformed into distinct electronic levels for electrons and holes, whose spacing can be simply tailored by the extent of the nanostructure. Hence, not only the semiconductor material for itself determines the colour of the emitted photons based on its individual band gap, also any structural size variation alters the optical properties.

For instance, nowadays light emitting diodes (LEDs) and laser diodes (LDs) for visible and ultraviolet light emission are predominantly based on group-III nitride heterostructures exhibiting a wurtzite crystal structure. All the advantages of this material system like an astonishing robustness, brilliance, and integrability come at the cost of a piezo- and pyroelectric polarisation along the natural [0001] growth direction. Generally, any stress-induced deformation of such polar crystals yields macroscopic charges at the crystal surfaces - a well known phenomenon for everyday devices like piezo ignition lighters. While the pyro-electricity is caused by the particular symmetry of the crystal, the piezoelectricity originates from strain evoked by hetero-interfaces of such materials with different lattice constants, altogether creating huge electrostatic fields (MV/cm) across the optically active regions. Hence, the beneficial confinement effect for electrons and holes is counterbalanced by a field-induced spatial separation, which spoils their pivotal overlap and ultimately the annihilation rate governing the light generation.

Here, we demonstrate that our Internal Field Guarded Active Region Design (IFGARD) is able to lock the polarisation fields out of any active region, while the polar and industrial most relevant growth direction is maintained, yielding a boost in electron-hole annihilation rates and therefore device efficiency by orders of magnitude. Previous attempts to tackle polarisation fields in affected materials did not reach industrial-relevance. Stabilizing the cubic phase of nitrides might be an approach of scientific elegance, however, the crystal quality deteriorates, turning the bright nitrides into rather dim emitters. Similarly, the realisation of numerous alternative growth directions of nitride materials can (partially) avoid the polarisation fields, but again suffers from a strongly reduced crystal quality besides additional technological challenges. In contrast, the IFGARD can bear on decades of research to improve the quality of strongly polar materials based on their most natural growth direction. The efforts to suppress any radiative as well as non-radiative losses has nowadays already led to record quantum efficiencies; a tedious and costly progression for polar material forming the basis for the IFGARD. Hence, our approach will combine the advantages of two worlds - well-established, high quality, polar material and high electron-hole pair annihilation rates.

In this article, the focus rests on two technologically most relevant types of nano heterostructures: two-dimensional quantum wells (QWs) and zero-dimensional quantum dots (QDs). Generally, the IFGARD does not only serve classical applications as LEDs and LDs, but will even break new ground for efficient and ultra-fast quantum light sources based on individual QDs.

Field guarding in quantum dots
The IFGARD is based on a simple, but at the same time counterintuitive idea. Commonly, the emissive, active material region (e.g. QD, QW) of devices features a smaller band gap than the matrix material in its surrounding providing the beneficial carrier confinement effect. In this situation, as exemplified in Fig. 1 a, any conventional device design strives to avoid additional layers that solely comprise the material of the active region to avoid light reabsorption. Hence, it appears as a ludicrous design to encapsulate this sandwich by the active region material as shown in Fig. 1 d. In this counterintuitive design a significant fraction of the emitted light gets reabsorbed by the, so-called, guard layers, casting doubt on the usability of the device - at first sight. However, guard material thicknesses below the emitted wavelength only absorb a well tolerable amount of emitted photons as discussed in the Supplementary Information (SI) - an effect that is by far overcompensated by the advantages of the IFGARD aiming to annihilate the detrimental, polarisation-induced, electric fields based on its particular design.
In order to exemplify the IFGARD, we first choose a GaN QD embedded in AlN - a selection that does not restrict the general applicability of the entire concept to a specific material system and/or nanostructure. *Figure 1* summarizes the major differences between a conventional GaN QD and its IFGARD counterpart in the first and second row, focussing from left to right on the composition, the polarisation fields, and the band structure. Here, the horizontal c-axis denotes the most favourable, natural [0001] growth direction of III-nitrides. *Fig. 1 a* shows a GaN QD with a height along this c-axis of 2 nm (dark grey) embedded in a matrix of AlN (light grey), while the IFGARD equivalent features thin AlN barriers and additional GaN guard layers as depicted in *Fig. 1 d*. A significant interface charge built-up occurs at the AlN/GaN/AlN interfaces, yielding a huge polarisation gradient with a potential drop of ≈ 1.7 V for the conventional case - right across the QD as shown in the colour-coded image of *Fig. 1 b*. Naturally, the associated polarisation potential overlays the band structure, provoking the band edges to be tilted right along the horizontal c-axis as shown in *Fig. 1 c*. As a result, not only a red-shift of the emission wavelength occurs, but also the electron and hole are spatially separated along the c-axis, lowering their overlap and subsequently the electron-hole pair annihilation rate. *Figure 1 e* illustrates this matter based on the electron (blue) and hole (red) density of states (profiles along the c-axis through the QD centre) and the corresponding overlap (coloured in green). The entire phenomenon that counteracts the confinement-induced blue-shift of the QD emission is known as the Quantum-Confined Stark Effect (QCSE) and has been studied in great profusion in the last decades. It is exactly this QCSE that researchers sought to overcome by e.g. stabilizing the cubic crystal structure phase or by realizing numerous alternative growth directions of III-nitrides.

Generally, the same charge built-up occurs for the IFGARD case depicted in *Fig. 1 d*. However, due to the inclusion of the guard layers, the polarisation potential gradient is now suspended from the QD. By adding two additional GaN/AlN interfaces as described by the IFGARD, one can suppress the electric field inside of the QD as depicted in *Fig. 1 e*. Here, the constant purple colouring of a major fraction of the QD corresponds to a suppression of the ionic potential gradient inside of the conventional QD structure separates the charge carriers as shown by the electron (blue) and hole (red) density of states in (c). In contrast, a drastically increased electron-hole overlap is obtained for the IFGARD QD (f) causing a beneficial boost in electron-hole oscillator strength and recombination rate.

![Figure 1](image)

**Figure 1 | IFGARD QD.** Comparison between a conventional quantum dot (QD) structure (1st row) and a QD comprising the Internal Field Guarded Active Region Design (IFGARD, 2nd row). From left to right: the particular layer sequence is exemplified for the GaN/AlN case as illustrated in the corresponding 2D-scans in (a) and (d). The contour-plots in (b) and (e) show the sum of the piezo- and pyroelectric potential for the conventional and the IFGARD QD structure. As a consequence of such particular potential distributions, different conduction and valence band edge profiles are obtained for a linear scan through the QD centre along the c-axis as depicted in (c) and (f). While the conventional QD structure exhibits a prominent potential gradient (yellow → black) inside of the QD (b), the IFGARD QD features a constant potential inside of the QD as evidenced by the purple colouring in (e). As a result, flat-band conditions are achieved inside of the IFGARD QD in contrast to a strong band-edge tilt for the conventional case (f, c). Consequently, the potential gradient inside of the conventional QD structure separates the charge carriers as shown by the electron (blue) and hole (red) density of states in (c). In contrast, a drastically increased electron-hole overlap is obtained for the IFGARD QD (f) causing a beneficial boost in electron-hole oscillator strength and recombination rate.
that are coloured accordingly.

Tailoring the internal field

The presented drastic changes regarding the emission characteristics are predominantly caused by the polarisation effects inherent to the crystal lattice and not by the influence of strain on the band structure - in this context an almost negligible,\textsuperscript{19}\textsuperscript{-21} but nevertheless still considered effect (see the SI for details). Therefore, we focus on the electric potential instead of the band edge profiles in order to illustrate the IFGARD effect in the following. Anihilating the QCSE by cancelling out the electric fields generated by the interface charges positioned on the opposite sides of the QD and barriers always exhibits the most tremendous effect. However, some fine tuning of the AlN barrier thicknesses is needed in order to reach a fully optimised field cancellation for QDs not only due to their top and bottom facets of different size but also due to their inclined side facets. Please note that these top and bottom facets correspond to the left and right GaN/AIN interface of the QD in Fig. 1 and 2 in order to allow a convenient comparison.

Figure 2 focuses on the influence of structural IFGARD parameters on the polarisation potential within another, here, 3-nm-high (h) QD shown in Fig. 2a. By varying the top AlN barrier thickness (t, red) above and the bottom barrier thickness (b, blue) below the QD, the gradient of the built-in electric potential drastically varies as plotted in Fig. 2b. By symmetrically decreasing both barrier widths (t = b), the potential gradient evolves from a drop (blue curve) within the QD for thick barriers (regarding a positive probe charge) to a corresponding rise for thinner barriers (red curve). AlN barrier thicknesses in between 1.5 nm and 2.0 nm (t = b) yield the smallest slopes for the potential trends as long as symmetric barriers are considered. However, the potential drop inside of the QD can be reduced even further if different barrier thicknesses are considered (t ≠ b). We find the combination of 1.5-nm- and 2.0-nm-thick AlN barriers to be ideal for reducing the absolute potential drop from the top to the bottom edge of the 3-nm-high IFGARD QD down to 5 mV. Interestingly, the inversion of the stack sequence (t ↔ b) does neither significantly alter the gradient, nor the particular trend for the electric potential, as evidenced by the black and green curves in Fig. 2b. Here, only the bottom barrier thickness regulates the absolute value of the potential inside of the QD in regard to an arbitrarily chosen zero. As soon as the flat-potential conditions are approached, a potential bowing becomes apparent originating from the piezo-electro polarization, which is caused by the particular strain distribution inside of the QD. It is of utmost importance to note that exactly the same 3-nm-high QD embedded in a conventional structure is affected by a total potential drop of -2112 mV as indicated in Fig. 2b (dashed, grey line) in contrast to the optimum of -5 mV. Therefore, we use exactly this straightforwardly accessible total potential drop (PD) as a convenient measure for the degree of internal field guarding due to the IFGARD.

Figure 2c plots PD values i.a. extracted from Fig. 2b following the applied colour coding. We derive a slope of -355 mV/nm for the PD values corresponding to the symmetric (t = b) barrier thickness increase (red to blue circles in Fig. 2c), whereas the sole increase of b (t = 1.5 nm) yields a slope of -173 mV/nm (black triangles in Fig. 2b). The inversion of the IFGARD stack (t ↔ b) does not significantly alter the PD value as indicated by the double triangle in Fig. 2c (green and black) and the potential scans in Fig. 2b that are coloured accordingly. Figure 2c proves the fact that both, negative and positive PD values are accessible by the presented concept allowing the IFGARD to reach the desirable flat-band condition (compare Fig. 1f) under any reasonable operating voltage in case of electrically driven devices.

Ultimately, the best barrier thickness constellations for the polarisation field guarding (t = 2.0 nm, b = 1.5 nm, or vice versa) boost the oscillator strength by a factor of 100 if compared to the conventional, 3-nm-high QD embedded in
AIN. In other words, the photon rate provided by each of such GaN QDs is increased by two orders of magnitude. Nevertheless, the advantages of the IFGARD even go beyond such a tremendous increase in overall QD brilliance. The absence of the QCSE for the IFGARD case in Fig. 1 d leads to a QD emission energy of 4.2 eV, which is now exclusively governed by the confinement, whereas the conventional QD from Fig. 1 a emits at 3.5 eV due to the red-shift induced by the additional QCSE. In direct comparison to the 50%-higher QD from Fig. 2 with emission energies of 2.9 eV and 4.0 eV, for the respective conventional and optimum IFGARD constellations, the QD size dependence of the emission energies is reduced by a factor of three from 3.5 eV - 2.9 eV = 0.6 eV to 4.2 eV - 4.0 eV = 0.2 eV. Hence, the energetically broad luminescence of conventional, e.g., nitride QD ensembles is minimized by the IFGARD. This is a fundamental prerequisite for any, e.g., laser application with a QD gain medium, as the QD dimensions will predominantly only affect their emission energy via the quantum confinement at the additional QCSE. In direct comparison to the 50% increase in crystal polarisation (plus and minus signs), a situation similar to stacked, parallel interfaces of different size occur in addition to less complex nano-wires. As the flat height in the band structure. Please see the SI for a variation of the QW composition.

Field guarding in quantum wells

After having exemplified the basic field-guarding concept and even its tunability for the case of QDs, we now come to an intuitive explanation regarding the functionality of the IFGARD based on the QW structure exemplified in Fig. 3 a. Here in this figure, the GaN IFGARD QD from Fig. 1 d got replaced by a GaN QW, again exhibiting a horizontal orientation of the polar c-axis. Similar to the QD case in Fig. 1 e, interface-charges build up at each of the GaN/AIN or AIN/GaN interfaces of the IFGARD QW structure as illustrated in Fig. 3 a by the + (red) or - (black) signs. Due to this particular, reverse interface sequence of the IFGARD it is now feasible to achieve flat-band conditions inside of this single-QW as shown in Fig. 3 b - top (black line) for a 2-nm-thick, single GaN QW encapsulated by two AIN barrier layers each with a thickness of t = b = 1 nm. In comparison, the conventional QW (h = 2 nm) illustrated by the red, dotted line in Fig. 3 b - top exhibits a pronounced band-structure inclination.

Already the fundamental symmetry of this QW IFGARD structure brings an intuitive analogy into mind - a stack of open-circuit, plate-type capacitors as depicted in Fig. 3 a. In this analogy, the distance between the capacitor plates corresponds to the thicknesses of the GaN QW and the AIN barriers. The crystal’s pyro- and piezoelectricity causes constant space charge densities at the interfaces of the IFGARD heterostructure similar to a charged, plate-type capacitor. Here, the central capacitor plates depicted in Fig. 3 a generate an electric field that can exactly be neutralized by the reversed field caused by the outer capacitor plates resulting in a field-free zone similar to the field-guarded interior of the IFGARD QW structure. Generally, the homogeneous electric field in between capacitor plates remains constant if their distance is varied and only the voltage ascribed to the potential difference in between the charged surfaces changes. In analogy, changing the thickness of the GaN QW or AIN barriers does not spoil the field-guarding effect as the relevant electric field superposition inside of the QW remains zero. Exactly the same observation is true for the electric field across a particular AIN barrier, which is in our analogy evoked by the charged, left or right plates of the inner and outer plate-type capacitor. Such a constant, non-zero electric field inside each of the AIN barriers is directly evidenced by a potential drop over a certain length interval in the corresponding band-structure calculations shown in Fig. 3 b and c. A constant slope of the band-structure trend (equivalent to constant electric fields) inside (non-zero) or outside (zero) of the AIN barriers is caused by the fixed space charges at all GaN/AIN and AIN/GaN interfaces evoked by pyro- and piezoelectricity. Interestingly, the analogy of stacked, open-circuit, plate-type capacitors facilitates a most simplistic understanding of QW IFGARD heterostructures as long as plan-parallel interfaces of infinite size are assumed.

The analogy gets into difficulties for the QD case as interfaces of different size occur in addition to less-polar QD side facets. Hence, any more complex nano-structure always requires the here applied numerical 3D-solution for the field situation as described in the SI in addition to all further simulation details. However, it is exactly the deviating interface geometry in the IFGARD QD structures that allows the tunability of the field inside of the QD by barrier thickness variations, cf. Fig. 2.

Generally, the fundamental IFGARD stack comprises exactly one barrier (e. g. AIN) along with one QW (e. g. GaN, sec. Fig. 3 a) and can arbitrarily be repeated (counted by n \in \mathbb{N}) without sacrificing the beneficial IFGARD effect seen in, e.g., Fig. 3 b - bottom for a 1-nm-thick double-QW. Such IFGARD QW stacking is neither limited by the number of

![Figure 3 | IFGARD QW](image-url)
Hence, the emission of each individual QD will not only separate, a most pivotal effect phonons wavefunction GaN or \([111]\) material channels formation of electron emission electron like saturation) increase the device’s emission intensity relies on pump power in population that decays with limited light emission density. Any, e.g., electrical carrier injection into the matrix material surrounding the QW(s) leads to an electron-hole pair population that decays with a polarisation-limited rate, while the device’s emission intensity relies on pump power in combination with a certain lateral size of the QW. Here, the main advantage of the IFGARD concept is the miniaturisation of lateral dimensions and the novel opportunity to further increase the pump power due to the enhanced device speed (no saturation), besides the aforementioned spectral narrowing of the emission. In contrast, as soon as smaller nanostructures like, e.g., zero-dimensional QDs are considered, a low electron-hole annihilation rate spoils the monochromatic emission as each QD must not be populated by more than one electron-hole pair. This, so-called, ground state exciton must decay with a rate that surpasses the QD fill rate. Otherwise, the formation of multi-excitons with deviating emission energies occurs. In this context, the IFGARD-enhanced recombination rate of the ground state exciton indirectly suppresses parasitic channels, which boosts the quantum efficiency.

Therefore, charge carriers should remain in the matrix material for a timeframe governed by the electron-hole annihilation rate, which, however, enables a strong influence of parasitic decay channels. Hence, the IFGARD concept is of utmost value as soon as polar QDs\(^{22,28}\) (e.g. \([0001]\)-wurtzite GaN or \([111]\)-zincblende InGaAs QDs) are considered, as both, the device speed and quantum efficiency can be raised. Generally, the boost in electron-hole pair annihilation rate by the IFGARD originates from an improved electron and hole wavefunction overlap that also reduces the electric dipole moment.\(^{27,28}\) As a direct consequence, the electrostatic coupling to charge fluctuations of nearby defects will be drastically reduced.\(^{4,29}\) At the same time, the coupling to phonons diminishes\(^{30,31}\) due to the reduced electron-hole separation, a most pivotal effect for electrically triggered, one- and two-photon sources\(^{22,26}\) operating up to room-temperature. Hence, the emission of each individual QD will not only become brighter, but also more energetically defined, and less temperature-sensitive.\(^{33}\) Such ultraviolet one- and two-photon sources represent an ideal candidate for the sub-diffraction analysis and nano-manipulation of extended molecules (DNA, RNA, etc.).\(^{34}\) Interestingly, the absorbance of these molecules\(^{35,36}\) nicely matches the emission range of GaN-based QDs\(^{37}\) enabling a strong perspective for individual bond cleavage\(^{8,19}\) based on one- and two-photon absorption if combined with optical near-field techniques\(^{40}\) in order to reach a spatial resolution that scales with the QD size only. IFGARD LEDs and LDs directly raise the question for an electrical contact and bipolar doping. Here, it can be of great advantage that the outer guard-layers of the IFGARD-based structure comprise the same material as the nanostructure in the active region. Electrical contacts and the bipolar doping of, e.g., GaN are nowadays straightforwardly achievable,\(^{24,41}\) whereas achievements of identical practicability are not yet accessible for AlN and cause excessive research efforts.\(^{42-46}\)

The electrical excitation of a single IFGARD QD is always based on a tunnelling process through the thin barrier layers comprising a material with a larger band gap. Therefore, the tunnelling probability is enhanced across the lateral extent of the QD and otherwise - in between the QDs - reduced due to the increased barrier thickness, cf. Fig. 2 a. In this sense, the IFGARD enables a current-channelling through the individual QDs, an effect that is otherwise achieved in single QD devices by complex processing of apertures.\(^{47}\) Please note that exactly the same effect is also relevant for extended structures like, e.g., one-dimensional quantum wires.

From a fundamental point of view, the IFGARD can beneficially be applied to all semiconductor combinations, which exhibit strong piezo- and/or pyroelectric fields. As a result, the (optical) characteristics of such next generation structures based on the IFGARD will no longer be predominantly affected by the QCSE as most frequently reported for III-nitride nanostructures.\(^{2,3,14,22,26-33}\) In general, the field-guarding conception boosts the radiative recombination and reduces the spectral emission width, while suppressing any parasitic recombination processes, an advantage that goes hand-in-hand with a strongly enhanced operation speed and a miniaturisation of highly efficient (quantum) light sources.

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1. Bimberg, D., Grundmann, M. & Ledentsov, N. N. Quantum dot heterostructures. (Wiley, 1998).
2. Gil, B. III-Nitride Semiconductors and Their Modern Devices. (Oxford University Press, 2013).
3. Ambacher, O. et al. Pyroelectric properties of Al(In)GaN/GaN hetero- and quantum well structures. J. Phys-Condens Mat 14, 3399–3434 (2002).
4. Kindel, C. et al. Spectral diffusion in nitride quantum dots: Emission energy dependent linewidths broadening via giant built-in dipole moments. Phys Stat Sol - Rapid Research Letters 8, 408–413 (2014).
5. Kako, S., Miyamura, M., Tachibana, K., Hashino, K. & Arakawa, Y. Size dependent radiative time decay of excitons in GaN/AlN self-assembled quantum dots. Appl Phys Lett 83, 984 (2003).
6. Pahn, G. M. O., Callsen, G. & Hoffmann, A. Internal field guarded active region device. German Patent Office (DPMA), ref: 102015217305.5.
7. Paisley, M. J. Growth of cubic phase gallium nitride by modified molecular-beam epitaxy. J. Vac. Sci. Technol. A 7, 701–705 (1989).
8. Maria Kemper, R. et al. Anti-phase domains in cubic GaN. J Appl Phys 110, 123512 (2011).
9. Bürger, M. et al. Lasing properties of non-polar GaN quantum dots in cubic aluminum nitride microdisk cavities. Appl Phys Lett 103, 021107 (2013).
20. Kako, S. et al. Single-photon emission from cubic GaN quantum dots. *Appl Phys Lett* 104, 011101 (2014).
21. Paskova, T. Nitrides with nonpolar surfaces: growth, properties, and devices. (Wiley, 2008).
22. Jiang, Y. et al. Realization of high-luminous-efficiency InGaN light-emitting diodes in the ‘green gap’ range. *Sci Rep* 5, 10883 (2015).
23. Han, J. & Kneissl, M. Non-polar and semipolar nitride semiconductors. *Semicond Sci Tech* 27, 020301 (2012).
24. Leroux, M. et al. Quantum confined Stark effect due to built-in internal polarization fields in (Al,Ga)N/GaN quantum wells. *Phys Rev B* 58, R13371–R13374 (1998).
25. Grandjean, N. et al. Built-in electric-field effects in wurtzite AlGaN/GaN quantum wells. *J Appl Phys* 86, 3714 (1999).
26. Nakaoka, T., Kako, S. & Arakawa, Y. Quantum confined Stark effect in single self-assembled GaN/AlN quantum dots. *Physica E* 32, 148–151 (2006).
27. Nakaoka, T., Kako, S. & Arakawa, Y. Unconventional quantum-confined Stark effect in a single GaN quantum dot. *Phys Rev B* 73, 121305 (2006).
28. Hönig, G. et al. Manifestation of unconventional biexciton states in quantum dots. *Nat Commun* 5, 5721 (2014).
29. Andreew, A. D. & O’Reilly, E. P. Optical transitions and radiative lifetime in GaN/AlN self-organized quantum dots. *Appl Phys Lett* 79, 521–523 (2001).
30. Andreew, A. D. & O’Reilly, E. P. Theory of the electronic structure of GaN/AlN hexagonal quantum dots. *Phys Rev B* 62, 15551 (2000).
31. Winkelkemper, M., Schliwa, A. & Binberg, D. Interrelation of structural and electronic properties in InGaN / GaN quantum dots using an eight-band kp model. *Phys Rev B* 74, 155322 (2006).
32. Kindel, C. et al. Exciton fine-structure splitting in GaN/AlN quantum dots. *Phys Rev B* 81, 245309 (2010).
33. Schliwa, A., Winkelkemper, M., Loechmann, A., Stock, E. & Binberg, D. In(Ga)As/GaAs quantum dots grown on a (111) surface as ideal sources of entangled photon pairs. *Phys Rev B* 80, 161307 (2009).
34. Mohan, A. et al. Polarization-entangled photons produced with high-symmetry site-controlled quantum dots. *Nature Photon* 4, 302–306 (2010).
35. Juska, G., Dimastromatano, V., Mereni, L. O., Gocalinska, A. & Pelucchi, E. Towards quantum-dot arrays of entangled photon emitters. *Nature Photon* 7, 527–531 (2013).
36. Callisen, G. et al. Steering photon statistics in single quantum dots: from one-to-two-photon emission. *Phys Rev B* 87, 245314 (2013).
37. Hönig, G. et al. Identification of electric dipole moments of excitonic complexes in nitride-based quantum dots. *Phys Rev B* 88, 045309 (2013).
38. Callisen, G. & Pahn, G. M. O. Identifying multi-excitions in quantum dots: the subtle connection between electric dipole moments and emission linewidths. *Phys Stat Sol (RRL) - Rapid Research Letters* 9, 521–525 (2015).
39. Ostapenko, I. A. et al. Large internal dipole moment in InGaN/GaN quantum dots. *Appl Phys Lett* 97, 063103 (2010).
40. Ostapenko, I. A. et al. Exciton acoustic-phonon coupling in single GaN/AIN quantum dots. *Phys Rev B* 85, 081303 (2012).
41. Callisen, G. et al. Analysis of the exciton-LO-phonon coupling in single wurtzite GaN quantum dots. *Phys Rev B* 92, 235439 (2015).
42. Holmes, M. J., Choi, K., Kako, S., Arita, M. & Arakawa, Y. Room-temperature triggered single photon emission from a III-nitride site-controlled nanowire quantum dot. *Nano Lett* 14, 982–986 (2014).
43. Kako, S. et al. A gallium-nitride single-photon source operating at 200K. *Nat Mater* 5, 887–892 (2006).
44. Howe, C. *Gene cloning and manipulation*. (Cambridge University Press, 2007).
45. Felsenfeld, G. & Hirschman, S. Z. A neighbor-interaction analysis of the hypochromism and spectra of DNA. *Journal of Molecular Biology* 13, 407–427 (1965).
46. Tataru, A. V., You, Y. & Owczarczyk, R. Predicting ultraviolet spectrum of single stranded and double stranded deoxyribonucleic acids. *Biophysical Chemistry* 133, 66–70 (2008).
47. Callisen, G. Advanced optical signatures of single, wurtzite GaN quantum dots. 1–171 (Technische Universität Berlin, 2015).
48. Schyma, P., Laaksonen, A. & Hugosson, H. W. Phosphodiester bond rupture in 5’ and 3’ cytosine monophosphate in aqueous environment and the effect of low-energy electron attachment: A Car–Parrinello QM/MM molecular dynamics study. *Chem Phys Lett* 462, 289–294 (2008).
49. Zheng, Y., Cloutier, P., Hunting, D. J., Wagner, J. R. & Sance, L. Phosphodiester and N-glucosidic bond cleavage in DNA induced by 4–15 eV electrons. *J Chem Phys* 124, 064710 (2006).
50. Betzig, E. & Trautman, J. K. Near-field optics: microscopy, spectroscopy, and surface modification beyond the diffraction limit. *Science* 257, 189–195 (1992).
51. Monemar, B. et al. Evidence for Two Mg Related Acceptors in GaN. *Phys Rev Lett* 102, 235501 (2009).
52. Callisen, G. et al. Optical signature of Mg-doped GaN: Transfer processes. *Phys Rev B* 86, 075207 (2012).
53. Morkoc, H. *Handbook of Nitride Semiconductors and Devices: Vol. 1: Materials Properties, Physics and Growth*. (Wiley, 2009).
54. Tang, Y.-B. et al. Tunable p-Type Conductivity and Transport Properties of AlN Nanowires via Mg Doping. *ACS Nano* 5, 3591–3598 (2011).
55. Peng, Y. et al. Tunable electronic structures of p-type Mg doping in AlN nanosheet. *J Appl Phys* 116, 044306 (2014).
56. Taniyasu, Y., Kasu, M. & Makimoto, T. An aluminium nitride light emitting nanosheet. *Acs Nano* 7, 328–332 (2006).
57. Unrau, W. et al. Electrically driven single photon source based on a site-controlled quantum dot with self-aligned current injection. *Appl Phys Lett* 101, 211119 (2012).
**Supplementary Information**

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**Methodical Overview**

It is the aim of this section to summarize our numerical procedure that facilitates the sophisticated, three-dimensional (3D) modelling for the particular case of quantum dots (QDs). Naturally, a principally equivalent, but one-dimensional (1D) method can trivially be applied to only two-dimensional structures like quantum wells (QWs). All calculations are based on an implementation of the 8-band-k·p formalism for wurtzite materials like nitrides, which is in detail described in literature and is further extended for the QD case by considering the particle interactions within the Hartree-Fock approximation. In the following we will provide a brief explanation for the entire set of complex calculations for the case of a QD as shown in Fig. S1.

A common simulation starts with the creation of, e.g., the 3D QD structure embedded in the matrix material (Fig. S1 a), whose size, shape, and chemical composition are specified on a finite-differences grid. All these individual properties of the particular nanostructures were extracted from atomic force microscopy analyses enabling a truly realistic description of such nanostructures. For the QD calculations we chose a mesh width of 0.1 nm in a box-shaped computation area - a value well below the actual monolayer spacing in e.g. GaN of ≈ 0.26 nm. A careful convergence behaviour analysis of all calculation results does not only confirm the chosen mesh width, but also the size of the calculation area of ≈ 30×30×30 nm³ (x×y×z) as adequate. Please note that such large calculation areas are problematic for any atomistic calculations but are essential in order to derive realistic (optical) properties in-line with various experimental results.

The differing crystal lattice parameters that originate from the varying chemical composition in the calculation area create a strain distribution that is iteratively calculated using a continuum mechanical model allowing a strain relaxation in the main growth direction known as the c-axis ([0001] direction). The resultant strain tensor distribution (e.g. ε_{zz} along the [0001] direction) is indicated in Fig. S1 b) affects the local electronic situation within and around the QD directly by strain-induced energy band deformations/shifts and indirectly by so-called piezoelectric polarizations. Subsequently, the calculation of the strain-dependent piezoelectric and the pyroelectric charge distributions inherent to the wurtzite structure is performed, evolving a corresponding electrostatic potential (see Fig. S1 c) as described by the basic Poisson equation.

Generally, the careful treatment of such electrostatic potentials is also of outstanding importance for materials that crystallize in the zinc-blende configuration - a most relevant fact for instance for InGaAs/GaAs QDs. Recently, the [111] growth direction has been a matter of intense research efforts dedicated to InGaAs/GaAs. Here, the application of the IFGARD concept could overcome the luminosity limitations of such [111]-based arsenide QDs, bringing their most prominent advantage for quantum photonics - a vanishing excitonic fine-structure splitting - to full bloom. Exactly in such arsenide materials, the second (quadratic) order of piezoelectricity has to be taken into account, while the spontaneous pyroelectricity inherent to nitrides is absent.

As soon as the electrostatic potential is known for the entire calculation area, one can straightforwardly create the Hamiltonian matrix values for each segment of the mesh. Applying the local 8×8 Hamiltonian matrix yields the coupling of the energetically lowest conduction band and the three topmost valence bands. Here, the previously derived electrostatic potential adds to the main diagonal of the 8×8 Hamiltonian. Furthermore, our Hamiltonian includes the effects of the spin-orbit and crystal-field coupling, which mainly affects the energy separations between the confined ground and excited hole states besides the band-mixing effects. A set of material parameters is utilized for the entire calculations as further described by Winkelkemper et al., whereas the sign of the piezoelectric constant ε₁₁ has been corrected as explained by Tomić et al. in reaction to the discussion in literature. All relevant parameters are summarized in Table S1. Solving the Schrödinger equation yields single-particle electron and hole envelope wavefunctions as depicted in Fig. S1 d) - a first, but rather inadequate description of an electron-hole pair because the inherent interactions are still neglected.

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**Figure S1| Simulations.** Calculation scheme for the applied 8-band k·p approach that yields the optical properties of the nanostructure of choice. (a) First, a nanostructure is defined before the strain distribution is continuum-mechanically calculated. The resulting ε_{zz} strain tensor component along the [0001] direction is exemplarily indicated in (b). Subsequently, the electrostatic potential (c) is derived considering the effects of pyro- and piezoelectricity of the specific crystal lattice. Solving the 8×8 Hamiltonian including the coupling of the energetically lowest conduction and the three highest valence bands - 4×2 bands due to the spin projections - yields single particle electron and hole envelope wavefunctions (d). An additional consideration of particle interactions (Coulomb and non-classical exchange interaction) generates converged electron-hole densities (d). Finally, the optical properties of such a two-particle state approximation are determined, yielding e.g. the oscillator strength of the corresponding, optical transition (f).
A more reasonable description of such a two-particle state known as an exciton is given by the mean field Hartree-Fock particle interaction approximation, yielding bound electron-hole densities shown in Fig. S1 e. Here, the Coulomb- and the non-classical exchange interactions between the electron and hole are iteratively calculated leading to a renormalisation of both wavefunctions for each iteration step until the total excitonic energy is converged. Finally, the optical transition properties of the exciton(s) formed by the converged electron and hole wavefunctions are determined as exemplified in Fig. S1 f. Previously, we have successfully applied this entire numerical procedure to an in detail analysis of polar and non-polar QDs in perfect agreement with numerous experimental results. Here, even an approximation of multi-excitions was recently derived based on the Configuration Interaction (CI) method, which yields non-separable wavefunctions. Generally, QD exciton simulations require a 3D description, while QW band edge calculations can sufficiently be described within a standard 1D approach, allowing a doubling of the simulation resolution. In summary, all our simulations describe the optical properties for the nanostructure of choice based on well-established procedures as directly approved by the experimental evidence - the supreme judge for modelling approaches.

### Stacking of field-guarded active regions

Generally, all modern LED and LD structures comprise extended layer stacks of various composition in order to boost significant parameters as charge carrier injection, light out-coupling, quantum efficiency, etc. - all aiming towards a maximisation of the most pivotal device luminosity. Hence, it is a question of special importance to clarify whether the IFGARD is generally compatible with such extended layer stacks without treating all optimizations required for an entire device.

In order to illustrate this matter, Fig. S2 shows the band edge profiles of two stacks of seven AlGaN/AlN QWs (each AlN barrier has a thickness of 0.25 nm in order to approximate one monolayer). While in Fig. S2 a all QWs still consist of pure GaN, the gallium-content is arbitrarily reduced in some of the QWs of Fig. S2 b in order to demonstrate the general capability of the IFGARD concept. Here, the composition variation leads to a band edge tilt within all QWs, which is representative for the individual gallium/aluminium ratio. Most intriguingly, both, positive and negative band edge inclinations can be achieved, independent of the individual QW thickness. As a result, the IFGARD enables new pathways for the design of highly unconventional potential landscapes as hinted in Fig. S2 b. Suddenly, the band edge inclination inside of the nanostructure becomes a tunable parameter that can either be addressed by composition (QW case, see Fig. S2 b) or by the individual implementation of the IFGARD (QD case, see Fig. 2). Nevertheless, any particular band edge engineering for devices with an externally applied bias remains a task for future work and goes well beyond the scope of the present manuscript.

By realizing such larger numbers of stacked IFGARD QWs, nanowires, or QDs the different refractive indices of the active region, the barrier, and the guard materials can even be utilized for planar mode-guiding approaches not only in, e.g., 1D and 2D photonic crystals, but also in basic edge-emitting lasers in order to further improve the specific light emission characteristics of the device. Here, only a sufficient thickness of the entire IFGARD stack must be reached in order to achieve any mode-guiding towards the, e.g., device’s side facets (perpendicular to the c-axis).

### Analysis of the technical feasibility

The growth of heterostructures that comprise QWs, quantum wires, or QDs along with numerous additional layers serving as Bragg reflectors, electron blocking layers, seed layers (polarity control), etc. is a well established procedure for many of the major, semiconductor compound families. Here, mainly the strongly polar oxide- and nitride-based correspondents often suffer from

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**Table S1 | Compilation of material parameters for GaN and AlN used for the one- and three-dimensional 8-band-k-p simulations.**

| Param. | GaN | AlN | Param. | GaN | AlN | Param. | GaN | AlN | Param. | GaN | AlN |
|--------|-----|-----|--------|-----|-----|--------|-----|-----|--------|-----|-----|
| $a_0$ (nm) | 0.3189 | 0.3112 | $e_\perp$ (Cm$^{-2}$) | -0.326 | -0.418 | $\Delta_{\text{B}}$ (eV) | 0.017 | 0.019 | $a_2$ (eV) | -11.3 | -11.8 |
| $c_0$ (nm) | 0.5185 | 0.4982 | $e_\parallel$ (Cm$^{-2}$) | -0.527 | -0.536 | $m_\perp/m_0$ | 0.186 | 0.322 | $D_1$ (eV) | -3.7 | -17.1 |
| $E_{1\parallel}$ (GPa) | 390 | 396 | $\epsilon_\parallel$ (Cm$^{-2}$) | 0.895 | 1.56 | $m_\parallel/m_0$ | 0.209 | 0.329 | $D_2$ (eV) | 4.5 | 7.9 |
| $E_{1\perp}$ (GPa) | 145 | 137 | $P_{\text{pyro}}$ (Cm$^{-2}$) | -0.034 | -0.090 | $E_{\text{P}}$ (eV) | 17.292 | 16.927 | $D_3$ (eV) | 8.2 | 8.8 |
| $E_{2\parallel}$ (GPa) | 106 | 108 | $\epsilon_\parallel$ | 9.8 | 9.1 | $E_p$ (eV) | 16.265 | 18.165 | $D_4$ (eV) | -4.1 | -3.9 |
| $E_{3\parallel}$ (GPa) | 398 | 373 | $E_f$ (eV) | 3.51 | 6.25 | $E_c$ (eV) | 0.8 | 0.0 | $D_5$ (eV) | -4.0 | -3.4 |
| $E_{4\parallel}$ (GPa) | 105 | 116 | $\Delta_{\text{B}}$ (eV) | 0.010 | -0.169 | $a_1$ (eV) | -9.4 | -3.4 | $D_6$ (eV) | -5.5 | -3.4 |

Figure S2 | Composition tuning. (a) The electric field guarding effect is maintained even for extended stacks of quantum wells (QWs) - here seven were chosen arbitrarily - as the flat-band conditions in the active region are still preserved. (b) Any composition variation in the QWs leads to a direct tunability of the immanent band structure inclination and step height. As a result, positive and negative band structure tilts become accessible independent of the individual QW thickness, only governed by the particular AlGaN composition. For simplicity we chose an AlN barrier thickness of 0.25 nm to approximate the thinnest possible structure of one monolayer.
large, inherent electric fields as they most preferentially crystallize in the wurtzite structure. Directly related, highly sophisticated heterostructures have been developed throughout the last decades and comprise extended layer stacks featuring smooth interfaces. Each of the layer thicknesses (guard layer, barrier, and QW) and, if applicable, QD geometries that were assumed for our demonstration of the IFGARD in Fig. 1 - 3 is straightforwardly achievable based on standard growth techniques as exemplified for the following section for the particular case of nitrides. Generally, such crystal polarisation is also highly relevant in (e.g. arsenide-based) cubic crystals. Here, the occurrence of piezoelectricity leads to similar detrimental effects if, e.g., the increasingly popular [111] growth direction is considered yielding major advantages for the generation of non-classical light based on QDs.\textsuperscript{5,17,20}

Growing IFGARD heterostructures based on e.g. nitride material can directly be achieved as long as all layers do not exceed the critical thickness for plastic relaxation, characteristic for the specific material system. Here, as an example, Fig. 2 assumes an AlN barrier thickness variation from 0.5 - 2.5 nm, well above the thickness of one monolayer and beneath the critical thickness of AlN grown on GaN of $\approx 3$ nm.\textsuperscript{40} Hence, as long as all layers are sufficiently thin, they are pseudomorphically strained and e.g. the growth of AlN on GaN is straightforwardly feasible, while the appearance of first cracks is reported for AlN thicknesses of 6 - 10 nm.\textsuperscript{5,14} At the same time, the inclusion of, e.g., GaN QWs is well feasible regarding the corresponding thickness range from Fig. 3 and also the growth of matching guard layers is straightforward. Here, two possible main device categories are accessible for the IFGARD concept. First, the IFGARD stack can be grown on, e.g., a bulk GaN substrate\textsuperscript{58} (bottom guard layer) and finally be capped by a sufficiently thin GaN layer (top guard layer) in order to ensure its optical transparency. Second, the entire IFGARD stack can be realized in a free-standing structure like, e.g., a nanobeam comprising a symmetric layer guard configuration with thicknesses scaling up to around 100 nm in order to achieve a sufficient mechanical stability of the final structure along with a reasonable optical transparency (see the following section). We would like to remark that the particular thickness of the guard layers provides quite a flexible option for tailoring an IFGARD-based device as it is only the occurrence of the additional interfaces that ensures the entire functionality as depicted in Fig. 3 a.

Naturally, at first sight, the IFGARD only favours the inclusion of QWs as they are most preferentially, pseudomorphically strained, in contrast to QDs whose growth process itself often relies on strain relaxation. Hence, the common, so called, Stranski-Krastanov (SK) growth mode of nitride QDs\textsuperscript{50,51} cannot straightforwardly be achievable in an IFGARD-based structure.\textsuperscript{52} Here, the rather thin and pseudomorphically strained AlN barrier layers (see Fig. 1 - 2) do not provide a sufficient lattice miss-match for SK QDs. Nevertheless, most recent studies on, e.g., GaN QD growth have shown that the underlying growth mechanism of such QDs can strongly deviate from the SK mode. Here, a desorption-driven growth mode was reported\textsuperscript{45} that does not rely anymore on common SK prerequisites, which is also true for the GaN QD nucleation close to structural defects.\textsuperscript{44} Also common droplet epitaxy\textsuperscript{45} can generate QD growth on pseudomorphically strained layers and is consequently well suited for any IFGARD QD device. Naturally, any electrical operation of the entire IFGARD structure is always based on charge carrier tunnelling through the sufficiently thin AlN barrier layers. Tremendous efforts of the last years were dedicated to the site-controlled growth of e.g. GaN QDs\textsuperscript{56} enabling novel optical applications in the ultraviolet spectral range as described in the main article. Here, several techniques exist like, e.g., the QD nucleation in etch pits,\textsuperscript{53} on nanowires,\textsuperscript{55} or on strain apertures,\textsuperscript{59} which all enable positioned, single QD(s) beyond the limits of a SK nucleation. In summary, all structural parameters for the active region (QWs and QDs), the barriers, and the guard layers that were assumed for a first demonstration of the IFGARD concept in Fig. 1 - 3 are highly realistic and are not even limited to a particular nanostructure type or material system.

Light absorption in the guard layers

At a first glance, the one and only apparent challenge of the IFGARD arises from the reabsorption of light in the guard layers as they comprise the same material as the active region in order to achieve flat-band conditions. Regarding the QD from Fig. 2 we showed that the electron-hole pair annihilation rate is increased by a factor of 100. This advantage is now partially counterbalanced by the light reabsorption in the guard layers. For an example we assume 50-nm-thick guard layers, which, even in a totally freestanding structure as known from one- and two-dimensional photonic crystals, still results in a mechanically stable nano-device.\textsuperscript{55,56} Hence, for typical GaN QD emission energies around 50% of the emitted light gets reabsorbed\textsuperscript{60} in the top guard-layer - a tolerable effect if compared to the increase in electron-hole annihilation rate by 100 for the ideal IFGARD configuration, cf. Fig. 2 b. However, please note that this first, simplistic estimation does not account for the Fabry-Pérot interferences that occur in the guard layer(s). The optical transparency of the guard layers for the particular QD emission wavelength ($\lambda$) exhibits a modulation governed by the guard layer thickness, exhibiting optima at $n \cdot \lambda / 8$ ($n \in \mathbb{N}$).\textsuperscript{51} However, such in detail design optimizations reside beyond the scope of this manuscript as also the characteristic radiation pattern of the QDs must be taken into account. Nevertheless, the trivial statement that any guard layer thickness of the order of the emitted wavelength enables sufficient transmission remains valid in consideration of the IFGARD benefits. Additionally, the light out-coupling along the c-axis can further be enhanced if the local density of optical states is altered based on a cavity structure as commonly applied for, e.g., nanobeam lasers.\textsuperscript{35}

1. Kindel, C. et al. Exciton fine-structure splitting in GaN/AlN quantum dots. Phys Rev B 81, 241309 (2010).
2. Haug, A. Theoretical solid state physics. (Pergamon, 1972).
3. Winkelkemper, M., Schliwa, A. & Bimberg, D. Interrelation of structural and electronic properties in InGaN / GaN quantum dots using an eight-band kp model. Phys Rev B 74, 155322 (2006).
4. Kindel, C., Kako, S., Kawano, T., Oishi, H. & Arakawa, Y. Collinear Polarization of Exciton/Biexciton Photoluminescence from Single Hexagonal GaN Quantum Dots. Jpn J Appl Phys 48, 04C116 (2009).
5. Kindel, C. H. Study on Optical Polarization in Hexagonal Gallium Nitride Quantum Dots. 1–194 (University of Tokyo, 2010).
6. Calis, G. et al. Analysis of the exciton-LO-phonon coupling in a wurtzite GaN quantum dot. Phys Rev B 92, 235439 (2015).
7. Lefebvre, P. et al. Observation and modeling of the time-dependent descreening of internal electric field in a wurtzite GaN: A0.15Ga0.85N quantum well after high photoexcitation. Phys Rev B 69, 035307 (2004).
8. Hönig, G. Mehrtelchenzustände in Halbleiter-Quantenpunkten. (Technische Universität Berlin, 2015).
9. Neugebauer, J. & Hickel, T. Density functional theory in materials science. WIREs Comput Mol Sci 3, 438–448 (2013).
10. Hönig, G. et al. Manifestation of unconventional biexciton states in quantum dots. Nat Commun 5, 5721 (2014).
11. Ostapenko, I. A. et al. Large internal dipole moment in InGaN/GaN quantum dots. Appl Phys Lett 97, 063103 (2010).
12. Borg, S. F. Matrix-tensor Methods in Continuum Mechanics. (Wspc, 1963).
13. Gil, B. Group III Nitride Semiconductor Compounds: Physics and Applications. (Clarendon Press, 1998).
14. Ambacher, O. et al. Pyroelectric properties of Al(In)GaN/GaN hetero- and quantum well structures. J Phys Condens Mat 14, 3399–3434 (2002).
15. Schlüter, A., Winkelkemper, M., Loichmann, A., Stock, E. & Bimberg, D. In(Ga)As/GaAs quantum dots grown on a (111) surface as ideal sources of entangled photon pairs. Phys Rev B 80, 161307 (2009).
16. Mohan, A. et al. Polarization-entangled photons produced with high-symmetry site-controlled quantum dots. Nature Photon 4, 302–306 (2010).
17. Juska, G., Dimassodronato, V., Mereni, L. O., Gocalsinska, A. & Peluchhi, E. Towards quantum-dot arrays of entangled photon emitters. Nature Photon 7, 527–531 (2013).
18. Bester, G., Wu, X., Vanderbilt, D. & Zunger, A. Importance of second-order piezoelectric effects in zinc-blende semiconductors. Phys Rev B 74, 081305 (2006).
19. Ehrhardt, M. & Kopyckni, T. Multi-Band Effective Mass Approximations: Advanced Mathematical Models and Numerical Techniques, chapter 2, 57-85 (Springer, 2014).
20. Gershoni, D., Henry, C. H. & Baraff, G. A. Calculating the optical properties of multidimensional heterostructures: Application to the modeling of quantum well lasers. IEEE J. Quantum Electron. 29, 2433–2450 (1993).
21. Rinke, P. et al. Consistent set of band parameters for the group-III nitrides AlN, GaN, and InN. Phys Rev B 77, 075202 (2008).
22. Vurgaftman, I. & Meyer, J. R. Band parameters for nitrogen-containing semiconductors. J Appl Phys 94, 3675–3696 (2003).
23. Winkelkemper, M. et al. Origin of the broad lifetime distribution of localized excitons in InGaN/GaN quantum dots. Phys Stat Sol B 245, 2766–2770 (2008).
24. Tomić, S. & Vukmirović, N. Excitonic and biexcitonic properties of single GaN quantum dots modeled by a-band kp theory and configuration-interaction method. Phys Rev B 86, 159902 (2012).
25. Pal, J., Tse, G., Haxha, V., Migliorato, M. A. & Tomić, S. Second-order piezoelectricity in wurtzite III-nitrogen semiconductors. Phys Rev B 84, 085211 (2011).
26. Schulz, S., Mourad, D., Schumacher, S. & Czyzch, G. Tight-binding model for the electronic and optical properties of nitride-based quantum dots. Phys Status Solidi B 248, 1853–1866 (2011).
27. Bastard, G. & Brum, J. A. Electronic states in semiconductor heterostructures. IEEE J. Quantum Electron. 22, 1625–1644 (1986).
28. Kindel, C. et al. Spectral diffusion in nitride quantum dots: Emission energy dependent linewidths broadening via giant built-in dipole moments. Phys Stat Sol - Rapid Research Letters 8, 408–413 (2014).
29. Hönig, G. et al. Identification of electric dipole moments of excitonic complexes in nitride-based quantum dots. Phys Rev B 88, 045309 (2013).
30. Callisen, G. & Pahn, G. M. O. Identifying multi-exciton interactions in quantum dots: the subtle connection between electric dipole moments and emission linewidths. Phys Stat Sol (RRL) - Rapid Research Letters 9, 521–525 (2015).
31. Nowozin, T. et al. Time-resolved high-temperature detection with single charge resolution of holes tunneling into many-particle quantum dot states. Phys Rev B 84, 075309 (2011).
32. Gil, B. Physics of Wurtzite Nitrides and Oxides: Passport to Devices. (Springer, 2014).
33. Gil, B. III-Nitride Semiconductors and Their Modern Devices. (Oxford University Press, 2013).
34. Triviño, N. V., Notte, R., Carlin, J.-F. & Grandjean, N. Continuous Wave Blue Lasing in III-Nitride Nanobeam Cavity on Silicon. Nano Lett 15, 1259–1263 (2015).
35. Vico Triviño, N. et al. High quality factor two dimensional GaN photonic crystal cavity membranes grown on silicon substrate. Appl Phys Lett 100, 071103 (2012).
36. Schmidt, G. et al. Nano-scale luminescence characterization of individual InGaN/GaN quantum wells stacked in a microcavity using scanning transmission electron microscopy cathode luminescence. Appl Phys Lett 105, 032101 (2014).
37. Kako, S. Optical Properties of Gallium Nitride Self-Assembled Quantum Dots And Application to Generation of Non-Classical Light. 1–271 (University of Tokyo, 2007).
38. Kako, S. et al. A gallium-nitride single-photon source operating at 200K. Nat Mater 5, 887–892 (2006).
39. Bykhovskih, A. D., Gelmont, B. L. & Shur, M. S. Elastic strain relaxation in GaN–AlN–Ga semiconductor–insulator–semiconductor structures. J Appl Phys 78, 3691 (1995).
40. Sanchez, A. M. et al. Critical thickness of high-temperature AlIN interlayers in GaN on sapphire (0001). J Electron Mater 30, L17–L20 (2001).
41. Koyama, T. et al. Strain-relaxation in NH 3-source molecular beam epitaxy of AlIN epilayers on GaN epitaxial templates. Phys Stat Sol (a) 203, 1603–1606 (2006).
42. Cao, Y. & Jena, D. High-mobility window for two-dimensional electron gases at ultrathin AlIN/GaN heterojunctions. Appl Phys Lett 90, 182112 (2007).
43. Dimitrakopoulos, G. P. et al. Strain relaxation in InGaN/GaN heterostructures grown by molecular beam epitaxy. Phys Stat Sol (a) 205, 2569–2572 (2008).
44. Leroux, M. et al. Quantum confined Stark effect due to built-in internal polarization fields in (Al,Ga)N/GaN quantum wells. Phys Rev B 58, R13371–R13374 (1998).
45. Grandjean, N. et al. Built-in-electric-field effects in wurtzite AlGaN/GaN quantum wells. J Appl Phys 86, 3714 (1999).
46. Lefebvre, P. et al. High internal electric field in a graded-width AlN/GaN quantum well: Accurate determination by time-resolved photoluminescence spectroscopy. Appl Phys Lett 78, 1252 (2001).
47. Hashimoto, T., Wu, F., Speck, J. S. & Nakamura, S. A GaN bulk crystal with improved structural quality grown by the ammonothermal method. Nat Mater 6, 568–571 (2007).
48. Sergent, S., Arita, M., Kako, S., Iwamoto, S. & Arakawa, Y. High-Q (>5000) AlN nanobeam photonic crystal cavity embedding GaN quantum dots. Appl Phys Lett 100, 121103 (2012).
49. Daudin, B. et al. Stranski-Krastanov growth mode during the molecular beam epitaxy of highly strained GaN. Phys Rev B 56, 7069 (1997).
50. Miyamura, M., Tachibana, K. & Arakawa, Y. High-density and size-controlled GaN self-assembled quantum dots grown by metalorganic chemical vapor deposition. Appl Phys Lett 80, 3937–3939 (2002).
51. Simeonov, D. et al. Strain relaxation of AlN epilayers for Stranski–Krastanov GaN/AlN quantum dots grown by metal organic vapor phase epitaxy. J Cryst Growth 299, 254–258 (2007).
52. Bellmann, K. et al. Desorption induced quantum dots on (0001) AlN by MOVPE. Phys Stat Sol (RRL) - Rapid Research Letters 9, 526–529 (2015).
53. Simeonov, D. et al. Evidence of size quantization effects in quantum dot emission from GaN islands formed at threading dislocations using nanoscale cathodoluminescence: A source of single photons in the ultraviolet. Appl Phys Lett 106, 252101 (2015).
54. Kawai, F. et al. GaN quantum-dot formation by self-assembling droplet epitaxy and application to single-electron transistors. Appl Phys Lett 79, 2243 (2001).
55. Holmes, M. et al. Measurement of an Exciton Rabi Rotation in a Single GaN/AlGaN Nanowire-Quantum Dot. Phys Rev Lett 111, 057401 (2013).
56. Yerino, C. D. et al. Strain-driven growth of GaAs(11) quantum dots with low fine structure splitting. Appl Phys Lett 105, 251901 (2014).
57. Bastard, M. J., Gram, K., Kako, S., Arita, M. & Arakawa, Y. Room-temperature triggered single photon emission from a III-nitride site-controlled nanowire quantum dot. Nano Lett 14, 982–986 (2014).
58. Unrau, W. et al. Electrically driven single photon source based on a site-controlled quantum dot with self-aligned current injection. Appl Phys Lett 101, 211119 (2012).
59. Muth, J. F. et al. Absorption coefficient, energy gap, exciton binding energy, and recombination lifetime of GaN obtained from transmission measurements. Appl Phys Lett 75, 2572–2574 (1999).
60. Chávez-Angel, E. et al. Reduction of the thermal conductivity in free-standing silicon nano-membranes investigated by non-invasive Raman thermometry. APL Mater. 2, 021113 (2014).