

## Article

# Polarization Engineered p-Type Electron Blocking Layer Free AlGa<sub>N</sub> Based UV-LED Using Quantum Barriers with Heart-Shaped Graded Al Composition for Enhanced Luminescence

Samadrita Das <sup>1</sup>, Trupti Ranjan Lenka <sup>1,\*</sup>, Fazal Ahmed Talukdar <sup>1</sup>, Hieu Pham Trung Nguyen <sup>2</sup> and Giovanni Crupi <sup>3</sup>

<sup>1</sup> Department of Electronics and Communication Engineering, National Institute of Technology Silchar, Silchar 788010, Assam, India; samadrita\_rs@ece.nits.ac.in (S.D.); fazal@ece.nits.ac.in (F.A.T.)

<sup>2</sup> Department of Electrical and Computer Engineering, Texas Tech University, 1012 Boston Avenue, Lubbock, TX 79409, USA; hieu.p.nguyen@ttu.edu

<sup>3</sup> BIOMORF Department, University of Messina, 98125 Messina, Italy; giovanni.crupi78@unime.it

\* Correspondence: trlenka@ieee.org

**Citation:** Das, S.; Lenka, T.R.; Talukdar, F.A.; Nguyen, H.P.T.; Crupi, G. Polarization Engineered p-Type EBL Free AlGa<sub>N</sub> Based UV-LED Using Quantum Barriers with Heart-Shaped Graded Al Composition for Enhanced Luminescence. *Micromachines* **2023**, *14*, 1926. <https://doi.org/10.3390/mi14101926>

Academic Editors: Julien Brault, Hao-Chung Kuo, Hsin-Chu Chen and Yi-Jen Chiu

Received: 26 August 2023

Revised: 3 October 2023

Accepted: 12 October 2023

Published: 13 October 2023



**Copyright:** © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

**Abstract:** In this paper, in order to address the problem of electron leakage in AlGa<sub>N</sub> ultra-violet light-emitting diodes, we have proposed an electron-blocking free layer AlGa<sub>N</sub> ultra-violet (UV) light-emitting diode (LED) using polarization-engineered heart-shaped AlGa<sub>N</sub> quantum barriers (QB) instead of conventional barriers. This novel structure has decreased the downward band bending at the interconnection between the consecutive quantum barriers and also flattened the electrostatic field. The parameters used during simulation are extracted from the referred experimental data of conventional UV LED. Using the Silvaco Atlas TCAD tool; version 8.18.1.R, we have compared and optimized the optical as well as electrical characteristics of three varying LED structures. Enhancements in electroluminescence at 275 nm (52.7%), optical output power (50.4%), and efficiency (61.3%) are recorded for an EBL-free AlGa<sub>N</sub> UV LED with heart-shaped Al composition in the barriers. These improvements are attributed to the minimized non-radiative recombination on the surfaces, due to the progressively increasing effective conduction band barrier height, which subsequently enhances the carrier confinement. Hence, the proposed EBL-free AlGa<sub>N</sub> LED is the potential solution to enhance optical power and produce highly efficient UV emitters.

**Keywords:** GaN; AlGa<sub>N</sub>; AlInN; ultra-violet (UV); electron blocking layer (EBL); light-emitting diode (LED); multi-quantum well (MQW)

## 1. Introduction

Due to the direct tunable band gap, between 3.43 eV and 6.11 eV, AlGa<sub>N</sub> ternary alloy is quite applicable to the fabrication of optical devices within a wavelength range of ~200–360 nm [1]. This is suitable for sterilization [2–5], ultra-violet printing [6,7], biomedical appliances [8,9], deodorization using a photo catalyst [10,11], dermatology in medicine [12,13], and sensing applications for materials, for example urea [14,15]. However, the internal quantum efficiency (IQE) and light output power (LOP) of UV-LEDs using AlGa<sub>N</sub> alloys are still low because of several adversities. Due to the overflow of electrons at high currents, the problem of efficiency drop occurs [16]. This happens because strong induced polarization fields and quantum-confined Stark effect (QCSE) [17] lead to a significant separation of electron and hole wave functions. Thus, there is a reduction of carrier confinement and radiative recombination in the quantum well of the

device.

To a certain extent, the overflow of electrons is eliminated by bringing a p-doped Al-rich electron blocking layer (EBL) between the multi-quantum well (MQW) and p-doped area [18]. However, the development of positively charged polarization sheet charges within the hetero-interface of the ultimate quantum barrier (QB) and EBL has a significant impact on the hole effectiveness [19,20]. Additionally, due to Al abundant EBL, magnesium doping efficiency is also impacted by high acceptor activation energy [21,22]. To mitigate the aforesaid challenges, various LED structures with re-designed EBL and QW have been addressed [23–27]. However, only a few challenges were able to be reduced, hence it is favorable to create EBL-free UV-LEDs resulting in an enhanced flow of carriers.

To tackle the difficulties caused by EBL, in this paper an EBL-free UV-LED with heart-shaped QBs has been presented operating at  $\sim 275$  nm wavelength. The conventional AlGaIn UV-LED consists of a thin intrinsic AlGaIn strip placed into the center of each QB. In our context, this design is modified with the utilization of heart-shaped QBs on the first five barriers. The heart-shaped graded Al composition-based UV LED shows the highest quantum efficiency and reduced efficiency drop due to the reduced polarization field and the elimination of the EBL layer in the device structure resulting from the progressively graded QBs. This unique LED structure offers a significantly reduced electrostatic field in the quantum well (QW) region due to the decreased lattice mismatch between the QW and the QB. Furthermore, the internal quantum efficiency of the proposed LED exhibits a massive enhancement due to the increased carrier confinement in the device active region and the reduced electron leakage to the p-type region resulted from the progressive increase in the effective conduction band barrier heights. Moreover, the hole injection efficiency of the proposed LED structures is greatly increased due to the reduced positive polarization sheet charges at the interface of the last QB and EBL, achieved later from the EBL. Consequently, the output power and wall-plug efficiency (WPE) of the proposed LED structure show significant enhancements compared to the conventional LEDs which are about 50.4% and 49.3%, respectively.

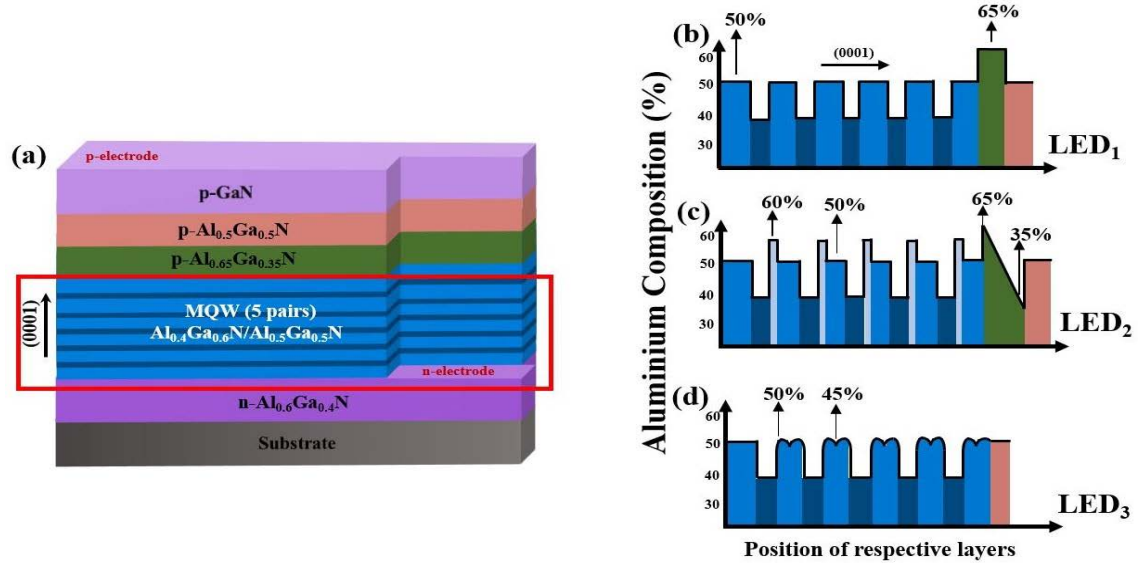
## 2. Structural Parameters

In this study, the performance of three distinct AlGaIn-based UV LED devices with non-identical MQWs and EBLs has been evaluated. To carry out the simulation, the ABC-model is used as the physical model for underlying the calculations. This model is based on the following assumptions: (i) carrier leakage from an LED structure's active region does not result in carrier losses, (ii) active region's non-equilibrium electron (n) and hole (p) concentrations are almost identical to one another, and (iii) carrier concentrations have a negligible impact on the recombination coefficients A, B, and C (details are explained below).

The deep ultra-violet LED fabricated by Yan et al. [28] is considered as the conventional device for reference (LED<sub>1</sub>) as shown in Figure 1a. The device has a dimension of  $400 \times 400 \mu\text{m}^2$  with  $\sim 275$  nm wavelength emission. An AlN buffer layer and 3  $\mu\text{m}$ -wide AlGaIn (60% Al; Si:  $5 \times 10^{18} \text{ cm}^{-3}$ ) layers are settled over the substrate. The following active region comprises of 5 periods of 10 nm thick intrinsic AlGaIn (50% Al) QBs and 3-nm-thick AlGaIn (40% Al) quantum wells (QWs), 20 nm thick p-Al<sub>0.65</sub>Ga<sub>0.35</sub>N EBL (Mg:  $2 \times 10^{19} \text{ cm}^{-3}$ ), succeeded by a 50 nm p-AlGaIn (50% Al) cladding layer (Mg:  $2 \times 10^{19} \text{ cm}^{-3}$ ), and finally a p-GaN contact layer of 120 nm width (Mg:  $1 \times 10^{20} \text{ cm}^{-3}$ ). The Al composition (%) profile in the active region and EBL related to the conduction band energy diagram of LED<sub>1</sub> is presented in Figure 1b.

As illustrated from the conduction band energy diagram in Figure 1c, LED<sub>2</sub> is constructed from LED<sub>1</sub> by replacing the uniform composition AlGaIn EBL with an Al<sub>x</sub>In<sub>1-x</sub>N layer which has a graded Al composition (x: 0.65–0.35). LED<sub>2</sub> includes a 3.5 nm Al<sub>0.6</sub>Ga<sub>0.4</sub>N single spike barrier and an 8.5 nm thick Al<sub>0.5</sub>Ga<sub>0.5</sub>N barrier in spite of the undoped AlGaIn barriers; excluding the first barrier which is nearest to the n-doped area.

The proposed device (LED<sub>3</sub>) in Figure 1d is finally realized by discarding the EBL and introducing graded Al composition to each of the heart-shaped barriers, with the exception of the first one. The remaining 10 nm intrinsic QBs are now composed of graded Al (x: 0.45–0.5–0.45–0.5–0.45) to form the heart-shaped structure.



**Figure 1.** (a) Schematic diagrams of LED<sub>1</sub>, Aluminum composition (%) related to the conduction band of (b) LED<sub>1</sub>, (c) LED<sub>2</sub>, and (d) LED<sub>3</sub>.

The electrical and optical characteristics of the device architectures are precisely recreated in this numerical analysis and studied with the help of commercially available industry-standard Silvaco ATLAS technology computer-aided design (TCAD).

In our work, we have used the Varshni formula to estimate the energy band gap of AlGa<sub>x</sub>N as follows [29]:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{\beta + T} \quad (1)$$

where  $\alpha$  and  $\beta$  represent material constants,  $E_g(0)$  and  $E_g(T)$  denote the energy band gap at 0, and  $T$  represents temperature, whose values are listed in Table 1 [30]. Equation (2) can be used to compute the band gap energy of Al<sub>x</sub>Ga<sub>1-x</sub>N using these values, as shown below [31]:

$$E(\text{Al}_x\text{Ga}_{1-x}\text{N}) = x \cdot E^{\text{AlN}} + (1 - x) \cdot E^{\text{Ga}} - b \cdot x \cdot (1 - x) \quad (2)$$

where  $b = 0.94$  is the bowing parameter, band-offset ratio is taken as 0.68/0.35 [31]. Constructing the band gap energy or band structures of the LEDs is an important step to understand the carrier transport, electron leakage, recombination mechanism, and electrostatic fields, which are explained in the following figures. These parameters are helpful in elucidating the performance of the devices, including quantum efficiency, wall-plug efficiency, and optical and electrical properties, which are presented and explained further.

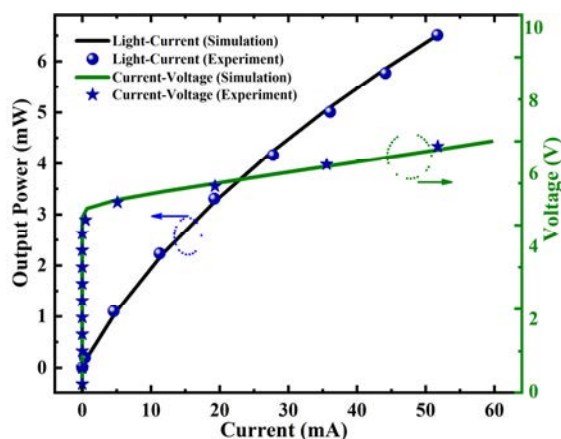
**Table 1.** Respective values of material constants for GaN, AlN [29].

Materials	$\alpha$	$\beta$	$E_g(0)$
GaN	0.919 meV/K	820 K	3.507 eV
AlN	1.789 meV/K	1432 K	6.23 eV

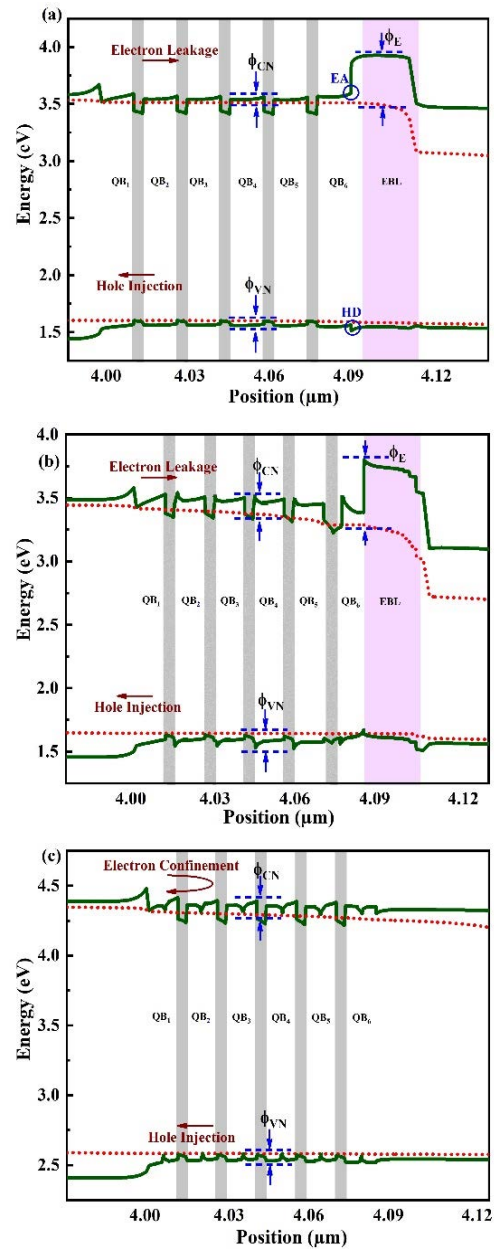
The energy band diagrams and carrier mobility are calculated using a  $6 \times 6$  k.p model [32] and the Caughey–Thomas approximation [33], respectively. The Shockley–Read–Hall (SRH), Radiative, and Auger recombination co-efficients are taken as  $6.67 \times 10^7/\text{s}$ ,  $2.13 \times 10^{-11} \text{ cm}^3/\text{s}$  and  $2.88 \times 10^{-30} \text{ cm}^6/\text{s}$ , respectively [34,35], and the SRH recombination lifetime is set to 15 ns. The light extraction efficiency is considered to be 15%. Moreover, the Mg activation energy varies across 165 meV to 515 meV for p-Al<sub>x</sub>Ga<sub>1-x</sub>N alloy [22]. From the methods of Fiorentini et al., the built-in polarization (spontaneous as well as piezoelectric) is estimated [36]. The entire simulation was carried out at a temperature of 300 K. The electron and hole mobilities are set to be  $100 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  and  $5 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  and other band parameters are available elsewhere [37].

### 3. Results and Discussion

With the use of experimentally obtained data from standard LED<sub>1</sub>, the device model, parameters, and tools employed in this work were optimized. The numerical simulation of the power-current-voltage graphs of LED<sub>1</sub> in Figure 2 closely matches the practically obtained curves, demonstrating the accuracy and dependability of our proposed design.

**Figure 2.** Measured and calculated light-current-voltage characteristics of LED<sub>1</sub> for model validation.

Then, numerical simulations on the electrical and optical properties of LED<sub>1</sub>, LED<sub>2</sub>, and LED<sub>3</sub> were carried out and the outcomes were compared one after another. Figure 3 illustrates the energy band diagrams (green solid lines) and quasi-Fermi levels (red dotted lines) of the three device samples at a 60 mA injected current. The variation in energy across the conduction/valence band and the quasi-Fermi levels is used to establish the efficient potential barrier heights for particles in the EBL ( $\phi_E$ ) and QBs ( $\phi_{CN}$ ). The optimum potential barrier height is acknowledged as the crucial factor in figuring out how to move the carrier. The corresponding values of  $\phi_{CN}$  and  $\phi_E$  are estimated from Figure 3a–c and listed in Table 2.



**Figure 3.** Estimated energy-band diagrams of (a) LED<sub>1</sub>, (b) LED<sub>2</sub>, and (c) LED<sub>3</sub> at an injection current of 60 mA. E.A and H.D are the electron accumulation region in the conduction band and hole depletion region in the valence band, respectively.

**Table 2.** Effective CBBH of barriers ( $\phi_{CN}$ ) and EBL ( $\phi_E$ ) for LED<sub>1</sub>, LED<sub>2</sub>, and LED<sub>3</sub>.

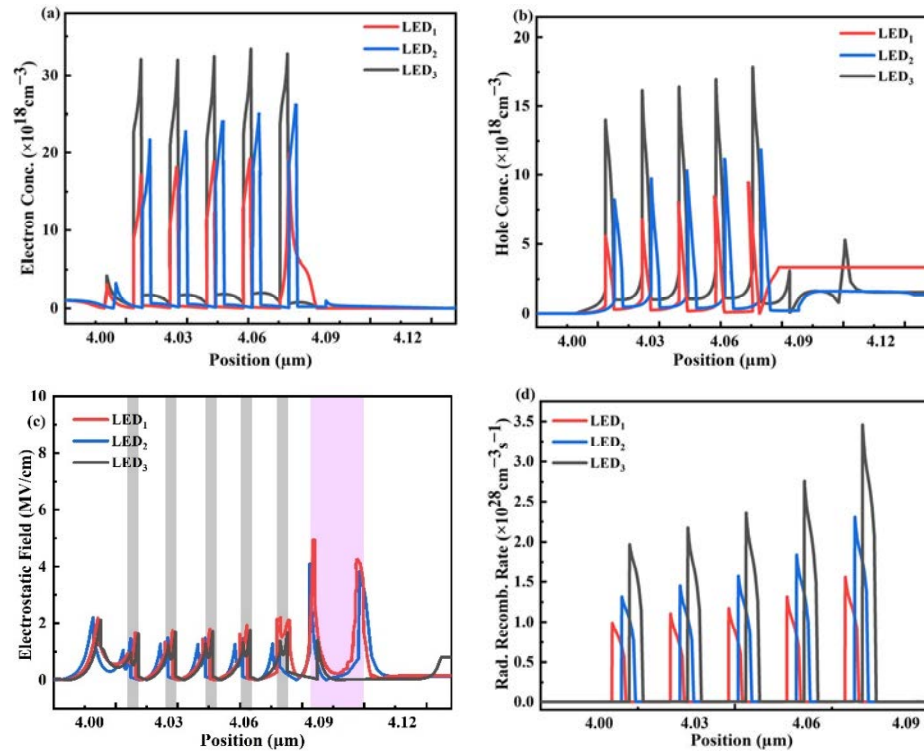
CBBH (meV)	LED <sub>1</sub>	LED <sub>2</sub>	LED <sub>3</sub>
$\phi_{C1}$	145.8	102.3	102.1
$\phi_{C2}$	164.4	110.7	109.1
$\phi_{C3}$	231.2	112.7	129.3
$\phi_{C4}$	298.1	115.9	194.0
$\phi_{C5}$	327.6	117.2	215.3
$\phi_{C6}$	249.8	121.4	311.9
$\phi_E$	244.1	256.0	

Hole injection efficiency in LED<sub>1</sub> is reduced by the hole depletion zone that forms as a result of polarization charge sheet contact across EBL/LQB. The  $\phi_E$  to prevent the excess of electrons in LED<sub>1</sub> is 244.1 meV, which is relatively low compared to the  $\phi_E$  and last QB height ( $\phi_{C6}$ ) of LED<sub>2</sub> and LED<sub>3</sub>. Due to the AlGaIn spikes in the first five barriers of LED<sub>2</sub>, a critical polarization field is generated due to high mismatch of lattices which reduces the CBBH and could possibly escalate the electron leakage. Nevertheless, in LED<sub>3</sub>, the heart-shaped graded QB results are in better match of the lattice. As a result, the polarization field has dropped and remarkably raised the CBBH, thus putting forward that the final LED design can prevent electron leakage to a great extent. Also, LED<sub>3</sub> shows a progressive growth in  $\phi_{CN}$  values while gradually increasing the amount of aluminum in the QBs. As a result, the electrons are resisted from jumping out of the wells and are confined within. Therefore, the hole injection into the active region increases while non-radiative recombination in the p-region decreases. The integration of heart-shaped graded Al composition in the middle of each QB supports the idea that the negative polarization sheet charges cause the creation of regions that are being accumulated by holes. Since LED<sub>3</sub> has the maximum CBBH, or  $\phi_{C6}$ , it is clear that LED<sub>3</sub> is the best option for containing electrons in the active zone. But a stronger electric field is produced in the active region of LED<sub>2</sub>, due to an extremely large lattice imbalance within the QBs and QWs, which has an impact on carrier containment. Moreover, Table 3 calculates and provides a list of the effective VBBH  $\phi_{VN}$  due to each QB. In comparison to LED<sub>1</sub>, LED<sub>2</sub>, and LED<sub>3</sub> have higher values of  $\phi_{VN}$ , which rises with the graded Al content of the QBs. This bolsters the enhanced hole concentration and better hole containment in the active region.

**Table 3.** Effective VBBH of barriers ( $\phi_{VN}$ ) for LED<sub>1</sub>, LED<sub>2</sub>, and LED<sub>3</sub>.

VBBH (meV)	LED <sub>1</sub>	LED <sub>2</sub>	LED <sub>3</sub>
$\Phi_{V1}$	225.2	302.3	252.1
$\Phi_{V2}$	224.7	317.1	261.7
$\Phi_{V3}$	223.1	329.0	272.4
$\Phi_{V4}$	222.2	362.3	289.6
$\Phi_{V5}$	221.9	372.1	294.2
$\Phi_{V6}$	220.3	384.6	309.5

Figure 4 show the three LEDs' carrier concentration, leak of electrons, and radiative recombination rate at 60 mA injection current. According to our analysis of Figure 4a, LED<sub>1</sub> shows a crucial electronic accumulation near the LQB/EBL junction and a significantly lower electronic concentration in the MQW. Additionally, all the QWs had a greater electron concentration due to LED<sub>3</sub>'s noticeably higher CBBH. According to Figure 4b, LED<sub>3</sub> had a higher concentration of holes in the QWs. This shows that both hole transfer and hole injecting efficiency have been improved as a result of the decreased VBBH in LED<sub>3</sub>.



**Figure 4.** Calculated (a) electron concentration, (b) hole concentration, (c) electrostatic field in the active region, and (d) radiative rate of recombination of three structures.

There is a strong electron accumulation in the well and barrier regions and minimal negative electrostatic field in LED<sub>3</sub>, because of which electron leakage is tremendously suppressed in the p-region, as shown in Figure 4c. The gray lines represent the QWs while the pink area signifies the EBL for LED<sub>1</sub> and LED<sub>2</sub>. With less chance of non-radiative combination of incoming holes with overflowing electrons, hole injection efficiency is increased. Also, as LED<sub>2</sub> has larger electron leakage, so the non-radiative recombination increases and the hole injection efficiency decreases.

The radiative recombination in all the QWs of LED<sub>3</sub> is higher, as displayed in Figure 4d, because of better overlap of the carrier wave functions [38], minimization of electron leakage, and betterment in hole efficiency [39].

In order to have a better understanding of the physical mechanism of enhanced electron confinement in our final device LED<sub>3</sub>, the electrostatic field in the active region is studied mathematically. The same can be estimated using the equations marked as (3)–(5) [40].

$$E_{QB} \approx \frac{t_{QW} \times \Delta P(w)}{t_{QW} \times \epsilon_{QB} + t_{QB} \times \epsilon_{QW}} \quad (3)$$

$$E_{QB} \times t_{QB} = E_{QW} \times t_{QW} \quad (4)$$

$$\Delta P(w) = \sigma_{interface} - \rho_{QB} \times w \quad (5)$$

$E_{QB}$  and  $E_{QW}$  are the electrostatic fields in QB and QW, respectively.  $\Delta P(w)$  denotes net polarization charge density along the growth direction 'w'.  $\epsilon_{QB}$  and  $\epsilon_{QW}$  represent dielectric constants of the barrier and well, respectively, and their respective widths are  $t_{QW}$  and  $t_{QB}$ . Because of the poor electrostatic field in the well, the electrons and holes are confined effectively [25]. Equation (4) depicts that  $E_{QB}$  and  $E_{QW}$  are directly proportional to each other. Also, from Equation (3),  $E_{QB}$  can be minimized by decreasing the

values of  $\Delta P(w)$  which is eventually connected to  $\sigma_{interface}$  and  $\rho_{QB}$ , as given in Equation (5). Again, using the following equations, the values of  $\sigma_{interface}$  and  $\rho_{QB}$  for LED<sub>2</sub> and LED<sub>3</sub> are measured and presented in Table 4. The polarization charge density at the  $QB_2/QW_2$  interlayer with respect to the spontaneous ( $P_{SP}$ ) and piezoelectric polarizations ( $P_{PP}$ ) is defined [41]. The equations are as follows:

$$\sigma_{interface} = [P_{SP}(QB) - \{P_{SP}(QW) + P_{PP}(QW)\}] \times 6.242 \times 10^{18} \quad (6)$$

$$P_{SP}(\text{Al}_x\text{Ga}_{1-x}\text{N}) = -0.09x - 0.034(1-x) + 0.019x(1-x) \quad (7)$$

$$P_{PP}(\text{Al}_x\text{Ga}_{1-x}\text{N}) = \{x \cdot P_{PP}(\text{AlN}) + (1-x) \cdot P_{PP}(\text{GaN})\} \cdot s \quad (8)$$

where,

$$P_{PP}(\text{AlN}) = -1.808 \cdot s + 5.624 \cdot s^2 (s < 0)$$

$$P_{PP}(\text{AlN}) = -1.808 \cdot s + 7.888 \cdot s^2 (s > 0)$$

$$P_{PP}(\text{GaN}) = -0.918 \cdot s + 9.541 \cdot s^2$$

$$\text{Basal strain, } s = \frac{QB_{LC} - QW_{LC}}{QW_{LC}}$$

The respective lattice constants (L.C) are found elsewhere [41]. The bulk charge density in the barriers, which is induced due to polarization, can be derived as shown in Equation (9) below:

$$\rho_{QB} = \frac{P_{SP}(\text{Al}_y\text{Ga}_{1-y}\text{N}) + P_{PP}(\text{Al}_y\text{Ga}_{1-y}\text{N}) - P_{SP}(\text{Al}_x\text{Ga}_{1-x}\text{N})}{w(y) - w(x)} \times 6.242 \times 10^{18} \quad (9)$$

where QB is graded from  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  to  $\text{Al}_y\text{Ga}_{1-y}\text{N}$ , and  $|w(y) - w(x)|$  is the grading distance. From Table 4,  $\sigma_{interface}$  is low in LED<sub>3</sub> compared to LED<sub>2</sub> because of the reduced lattice mismatch at the interfaces. However,  $\rho_{QB}$  values are high in LED<sub>3</sub> due to the graded configuration of the Al content. As a whole,  $\Delta P(w)$  is low in LED<sub>3</sub> which leads to a poor electrostatic field in each QB. This, in turn, also reduces the electrostatic field in the QW. Figure 4c also predicts a lower electrostatic field in the MQW of LED<sub>3</sub>, due to which carrier confinement is enhanced in LED<sub>3</sub>.

**Table 4.** Calculated  $\sigma_{interface}$  at QB/QW interface, and  $\rho_{QB}$  in the barriers of LED<sub>2</sub> and LED<sub>3</sub>.

LED	$\sigma_{interface} (\times 10^{16})$				$\rho_{QB} (\times 10^{17})$			
	$QB_2/QW_2$	$QB_3/QW_3$	$QB_4/QW_4$	$QB_5/QW_5$	$QB_2$	$QB_3$	$QB_4$	$QB_5$
LED <sub>2</sub>	4.789	5.876	6.983	8.112	3.535	3.565	3.599	3.636
LED <sub>3</sub>	4.078	5.149	6.242	7.356	3.554	3.588	3.624	3.659

The IQE, LOP, current-voltage (I-V) characteristics, and electroluminescence (EL) intensity of the three LEDs are illustrated in Figure 5. The following equations establish the structure's current density ( $j$ ) and its IQE using the ABC-model.

$$\frac{j}{qd} = An + Bn^2 + Cn^3 \quad (10)$$

$$IQE = \frac{Bn}{A + Bn + Cn^2} \quad (11)$$

$q$  = charge of electron,  $A = 1/\tau$  ( $\tau$  = Shockley–Read non-radiative carrier lifetime),  $B$  = radiative recombination constants,  $C$  = Auger recombination constants,  $d$  = effective width of the recombination region. The calculated maximum IQEs for LED<sub>1</sub>, LED<sub>2</sub>, and LED<sub>3</sub> are 39.3%, 47.7%, and 55.3%, respectively, as shown in Figure 5a, indicating that the effi-



ciency of LED<sub>3</sub> is 40.7% and 15.9% larger than that of LED<sub>1</sub> and LED<sub>2</sub>, respectively. Additionally, from the inset of Figure 5a, at 60 mA injection current, the efficiency drop of LED<sub>3</sub> is noticeably reduced to 2.53%.

From Figure 5b, the optical power of LED<sub>3</sub> is remarkably increased (~17.3 mW) at a 60 mA current, which is 61.7% better compared to the conventional device. They are attributed to improved carrier transit and confinement in the MQW, greater electron and hole wave function overlap, reduced electron leakage, and improved hole injection efficiency.

As displayed in Figure 5c, all three structures have a nearly equal turn-on voltage. It is also noticeable that at a 60 mA current, LED<sub>3</sub> exhibits a slightly higher operating voltage because of the heart-shaped QBs and also due to the absence of EBL.

The constant analytical dependence of the anticipated IQE on the radiative current density ( $j_{rad}$ ) is a further significant characteristic of the ABC model, as shown in Equation (12).

$$IQE = \frac{Q}{Q + \left(j_{rad}/j_m\right)^{\frac{1}{2}} + \left(j_{rad}/j_m\right)^{-\frac{1}{2}}} \quad (12)$$

$Q$  = quality factor which is independent of current density and equal to  $B(\tau/C)^{1/2}$  within the ABC-model. Radiative recombination rates cause the value of  $Q$  to rise while the Auger and Shockley–Read recombination rates cause it to fall. Furthermore, the magnitude of  $Q$  solely determines how dependent the IQE is on the  $j_{rad}/j_m$  ratio ( $j_m = qdB/\tau C$  within the ABC-model). As a result, this value may be used as a measure of merit for LED structures with varied designs, or those that emit light in diverse spectral regions.

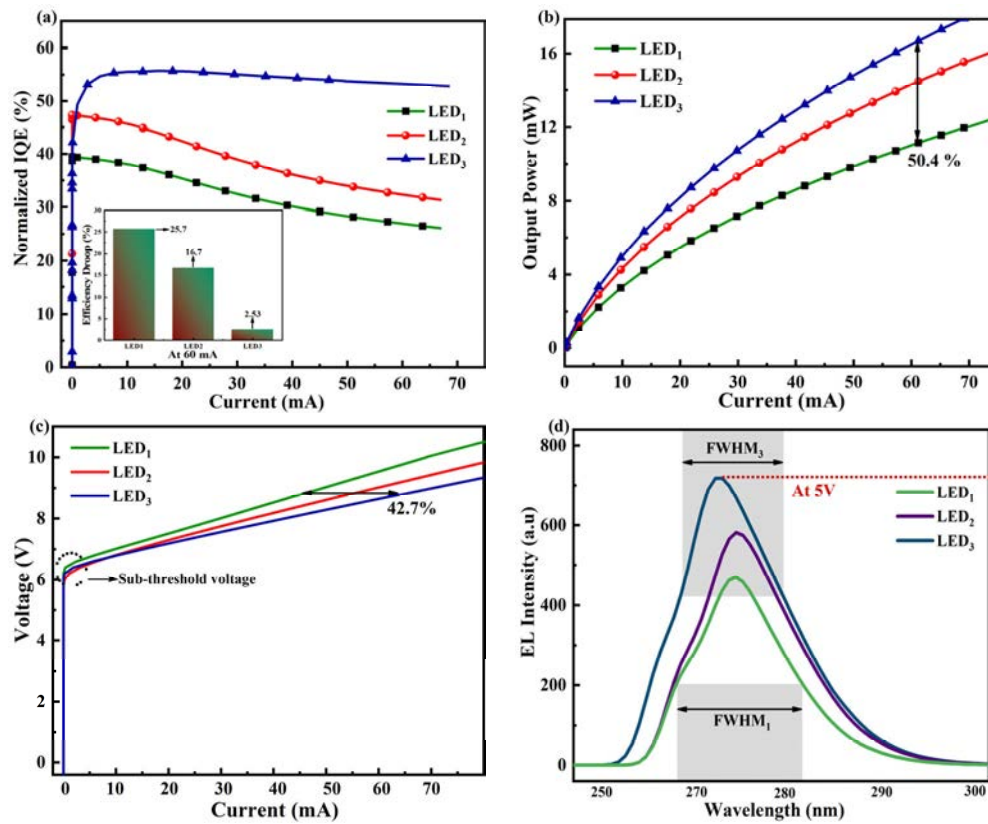
According to Figure 6, the analytical dependence (12) accurately reproduces the IQE variation with current density in the structures of different LED designs. It is discovered that the specific value of the quality factor given in each plot correlates with both the maximum efficiency and its decline with current. This factor varies from 0.78 to 18, depending on how well each structure's design and construction materials perform overall.

For clear comparison, the calculated parameters of IQE, LOP, and efficiency drop of the three samples are summarized in Table 5.

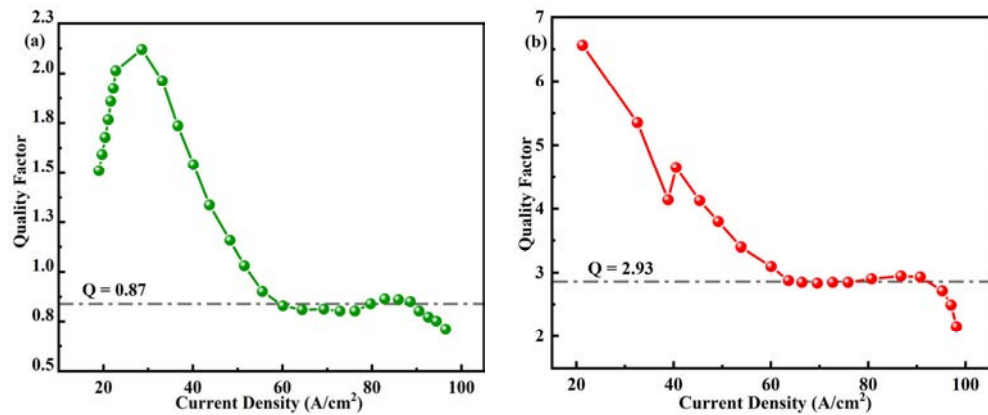
**Table 5.** Optimized performance parameters for LED<sub>1</sub>, LED<sub>2</sub>, and LED<sub>3</sub>.

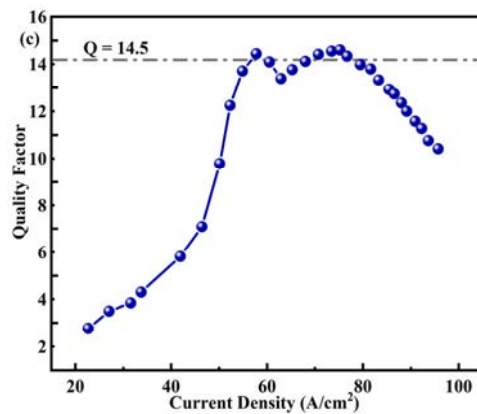
Parameters	LED <sub>1</sub>	LED <sub>2</sub>	LED <sub>3</sub>
Maximum IQE (%)	39.3 at 1.93 mA	47.7 at 3.28 mA	55.3 at 2.78 mA
IQE (%) at 60 mA	29.2	40.9	53.9
Efficiency Droop (%) at 60 mA	25.7	16.7	2.53
Luminous Power at 60 mA (mW)	10.7	13.9	17.3

Due to better radiative recombination and lower leakage of electrons, LED<sub>3</sub> displays dominant EL intensity at an emission wavelength of ~275 nm, as shown in Figure 5d. EL intensity of LED<sub>3</sub> is ~1.52 times higher than LED<sub>1</sub> and ~1.23 times higher than LED<sub>2</sub>. Peak fitting is used to calculate the full width at half maximum (FWHM) of each spectrum, as illustrated in Figure 5d. The combined impacts of the larger efficient hole injection and the better capability of heart-shaped graded Al Composition in the QBs are responsible for the superiority. Strong electron confinement in the QW of LED<sub>3</sub> causes it to emit a relatively sharp and narrow light beam. As an outcome it has a small spectral width and FWHM. LED<sub>1</sub>, in comparison, has substantially wider radiation patterns (beam width), which result in wider FWHM and wide spectral bands.



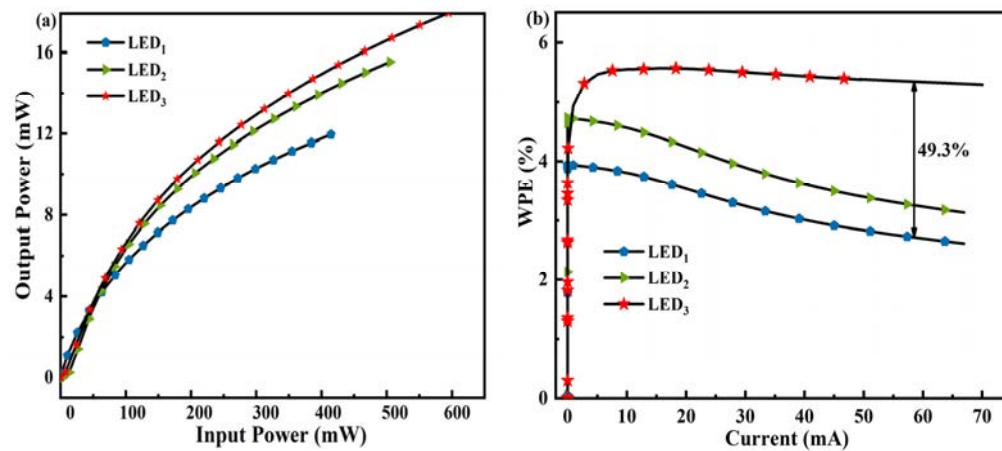
**Figure 5.** Measured (a) Efficiency, (b) Luminous Power, (c) I-V, and (d) EL intensity properties of LED<sub>1</sub>, LED<sub>2</sub>, and LED<sub>3</sub>.





**Figure 6.** Quality factor as a function of current density obtained from the data reported for (a) LED<sub>1</sub>, (b) LED<sub>2</sub>, and (c) LED<sub>3</sub>.

From Figure 7a, the optical output power of LED<sub>3</sub> is immensely raised along with input power supply. Also, the contrasting results of controlling the input supply in the devices is primarily ascribed to varying operational bias, as shown in Figure 5c. Figure 7b displays the wall-plug efficiency (WPE) as a factor of input current for each LED structure. The WPE of LED<sub>3</sub> is ~5.39% at 60 mA, which is enhanced by nearly ~49.3% compared to LED<sub>1</sub>. The increased output power of our suggested device LED<sub>3</sub> is what gives it a better WPE. For better understanding, the performance parameters of our work have been compared to the recent research works and their approximate values are listed in Table 6.



**Figure 7.** Approximated (a) output power with respect to input power, (b) WPE vs. injected current of LED<sub>1</sub>, LED<sub>2</sub>, and LED<sub>3</sub>.

**Table 6.** Comparison of performance metrics with recent research works.

Author	Maximum IQE (%)	Droop (%)	Power (mW)	References
Kang et al.	27.51	3.01	8.24	[42]
Jain et al.	35.17	20.68	13.9	[43]
Velpula et al.	5.3	9.1	15.68	[44]
Ji et al.	9.16	11.24	16.11	[45]
Pandey et al.	4.12	19.21	8.91	[46]
This work	53.9	2.53	17.3	

#### 4. Conclusions

We have explored and reported the effect of UV LEDs with heart-shaped QBs and no EBLs across a wavelength range of ~275 nm. The parameters utilized are taken from the data of the experimental reference device in order to verify the validity of the simulation results. The proposed device has an emitting layer thickness of >30 nm due to which the long-life stability is 90,000 h. These simulated results reveal that incorporating the proposed QB is advantageous for achieving high optical output power and WPE in the UV spectral range. The p-EBL free device can effectively suppress the excess flow of electrons and support a boosted hole injection. The EBL-free structure is also advantageous from the perspective of epitaxial growth because it prevents the development of p-heavy doped Al composition in the EBL. This, in turn, reduces the device resistance. The proposed structure records output power of 16.1 mW and displays increased radiative recombination, IQE of 53.9% at 60 mA which is larger than the remaining structures by 1.5 and 1.8 times, respectively. Therefore, the reported LED structure shows great potential and has the ability to produce UV LEDs with significant performances for various utilities in the practical world.

**Author Contributions:** S.D.: Conceptualization, Design, Simulation and Writing of manuscript; T.R.L.: Conceptualization, Supervision, Writing—review and editing and Funding; F.A.T.: Supervision, Writing—review and editing; H.P.T.N.: Supervision, Writing—review and editing; G.C.: Supervision, Writing—review and editing. All authors have read and agreed to the published version of the manuscript.

**Funding:** This study was funded by DST-SERB: Government of India sponsored MATRICS Project No. MTR/2021/000370 and US National Science Foundation, under grant number 1944312.

**Data Availability Statement:** The data and materials may be available on request basis.

**Acknowledgments:** This work is the outcome of DST-SERB, Govt. of India sponsored MATRICS Project No. MTR/2021/000370 which is duly acknowledged for kind support. H. P. T. Nguyen also acknowledges financial support from the US National Science Foundation, under grant number 1944312.

**Conflicts of Interest:** The authors declare no conflicts of interest.

#### References

1. Muramoto, Y.; Kimura, M.; Nouda, S. Development and future of ultraviolet light-emitting diodes: UV-LED will replace the UV lamp. *Semicond. Sci. Technol.* **2014**, *29*, 084004. <https://doi.org/10.1088/0268-1242/29/8/084004>.
2. Gassie, L.W.; Englehardt, J.D. Advanced oxidation and disinfection processes for onsite net-zero greywater reuse: A review. *Water Res.* **2017**, *125*, 384–399. <https://doi.org/10.1016/j.watres.2017.08.062>.
3. Zhou, X.; Li, Z.; Lan, J.; Yan, Y.; Zhu, N. Kinetics of inactivation and photoreactivation of Escherichia coli using ultrasound-enhanced UV-C light-emitting diodes disinfection. *Ultrason. Sonochem.* **2017**, *35*, 471–477. <https://doi.org/10.1016/j.ultsonch.2016.10.028>.
4. Rattanakul, S.; Oguma, K. Analysis of Hydroxyl Radicals and Inactivation Mechanisms of Bacteriophage MS<sub>2</sub> in Response to a Simultaneous Application of UV and Chlorine. *Environ. Sci. Technol.* **2017**, *51*, 455–462. <https://doi.org/10.1021/acs.est.6b03394>.
5. Rattanakul, S.; Oguma, K. Inactivation kinetics and efficiencies of UV-LEDs against Pseudomonas aeruginosa, Legionella pneumophila, and surrogate microorganisms. *Water Res.* **2018**, *130*, 31–37. <https://doi.org/10.1016/j.watres.2017.11.047>.
6. Okamura, H.; Niizeki, S.; Ochi, T.; Matsumoto, A. UV curable formulations for UV-C LEDs. *J. Photopolym. Sci. Technol.* **2016**, *29*, 99–104. <https://doi.org/10.2494/photopolymer.29.99>.
7. Okamura, H.; Matoba, T.; Takada, K.; Yamashita, M.; Shirai, M.; Matsumoto, A. Photo-thermal dual curing of acrylic anchor resins for screen printing. *Prog. Org. Coat.* **2016**, *100*, 47–50. <https://doi.org/10.1016/j.porgcoat.2016.01.025>.
8. Yamazaki, S.; Nishioka, A.; Kasuya, S.; Ohkura, N.; Hemmi, H.; Kaisho, T.; Taguchi, O.; Sakaguchi, S.; Morita, A. Homeostasis of Thymus-Derived Foxp3<sup>+</sup> Regulatory T Cells Is Controlled by Ultraviolet B Exposure in the Skin. *J. Immunol.* **2014**, *193*, 5488–5497. <https://doi.org/10.4049/jimmunol.1400985>.
9. Nakamura, M.; Morita, A.; Seit , S.; Haarmann-Stemmann, T.; Grether-Beck, S.; Krutmann, J. Environment-induced lentigines: Formation of solar lentigines beyond ultraviolet radiation. *Exp. Dermatol.* **2015**, *24*, 407–411. <https://doi.org/10.1111/exd.12690>.
10. Fujishima, A.; Zhang, X. Titanium dioxide photocatalysis: Present situation and future approaches. *Comptes Rendus Chim.* **2006**, *9*, 750–760. <https://doi.org/10.1016/j.crci.2005.02.055>.

11. Nakata, K.; Fujishima, A.  $\text{TiO}_2$  photocatalysis: Design and applications. *J. Photochem. Photobiol. C Photochem. Rev.* **2012**, *13*, 169–189. <https://doi.org/10.1016/j.jphotochemrev.2012.06.001>.
12. Das, S.; Lenka, T.R.; Talukdar, F.A.; Velpula, R.T.; Jain, B.; Nguyen, H.P.T.; Crupi, G. Effects of polarized-induced doping and graded composition in an advanced multiple quantum well InGaN/GaN UV-LED for enhanced light technology. *Eng. Res. Express* **2022**, *4*, 015030. <https://doi.org/10.1088/2631-8695/ac4fb1>.
13. Khan, M.A.; Shatalov, M.; Maruska, H.P.; Wang, H.M.; Kuokstis, E. III-nitride UV devices. *Jpn. J. Appl. Phys.* **2005**, *44*, 7191–7206. <https://doi.org/10.1143/JJAP.44.7191>.
14. Uhlin, F.; Fridolin, I.; Lindberg, L.G.; Magnusson, M. Estimating total urea removal and protein catabolic rate by monitoring UV absorbance in spent dialysate. *Nephrol. Dial. Transplant.* **2005**, *20*, 2458–2464. <https://doi.org/10.1093/ndt/gfi026>.
15. Tomson, R.; Uhlin, F.; Fridolin, I. Urea rebound assessment based on UV absorbance in spent dialysate. *ASAIO J.* **2014**, *60*, 459–465. <https://doi.org/10.1097/MAT.0000000000000091>.
16. Cho, J.; Schubert, E.F.; Kim, J.K. Efficiency droop in light-emitting diodes: Challenges and counter measures. *Laser Photonics Rev.* **2013**, *7*, 408–421. <https://doi.org/10.1002/lpor.201200025>.
17. Pieniak, K.; Chlipala, M.; Turski, H.; Trzeciakowski, W.; Muziol, G.; Staszczak, G.; Kafar, A.; Makarowa, I.; Grzanka, E.; Grzanka, S.; et al. Quantum-confined Stark effect and mechanisms of its screening in InGaN/GaN light-emitting diodes with a tunnel junction. *Opt. Express* **2021**, *29*, 1824. <https://doi.org/10.1364/oe.415258>.
18. Hirayama, H.; Fujikawa, S.; Noguchi, N.; Norimatsu, J.; Takano, T.; Tsubaki, K.; Kamata, N. 222–282 nm AlGaIn and InAlGaIn-based deep-UV LEDs fabricated on high-quality AlN on sapphire. *Phys. Status Solidi* **2009**, *206*, 1176–1182. <https://doi.org/10.1002/pssa.200880961>.
19. Chu, C.; Tian, K.; Che, J.; Shao, H.; Kou, J.; Zhang, Y.; Li, Y.; Wang, M.; Zhu, Y.; Zhang, Z.-H. On the origin of enhanced hole injection for AlGaIn-based deep ultraviolet light-emitting diodes with AlN insertion layer in p-electron blocking layer. *Opt. Express* **2019**, *27*, A620. <https://doi.org/10.1364/oe.27.00a620>.
20. Velpula, R.T.; Jain, B.; Bui, H.Q.T.; Shakiba, F.M.; Jude, J.; Tumuna, M.; Nguyen, H.-D.; Lenka, T.R.; Nguyen, H.P.T. Improving carrier transport in AlGaIn deep-ultraviolet light-emitting diodes using a strip-in-a-barrier structure. *Appl. Opt.* **2020**, *59*, 5276. <https://doi.org/10.1364/ao.394149>.
21. Nakarmi, M.L.; Nepal, N.; Lin, J.Y.; Jiang, H.X. Photoluminescence studies of impurity transitions in Mg-doped AlGaIn alloys. *Appl. Phys. Lett.* **2009**, *94*, 10–13. <https://doi.org/10.1063/1.3094754>.
22. Nam, K.B.; Nakarmi, M.L.; Li, J.; Lin, J.Y.; Jiang, H.X. Mg acceptor level in AlN probed by deep ultraviolet photoluminescence. *Appl. Phys. Lett.* **2003**, *83*, 878–880. <https://doi.org/10.1063/1.1594833>.
23. Zhang, Z.H.; Chen, S.-W.H.; Chu, C.; Tian, K.; Fang, M.; Zhang, Y.; Bi, W.; Kuo, H.-C. Nearly efficiency-droop-free algaIn-based ultraviolet light-emitting diodes with a specifically designed superlattice P-type electron blocking layer for high MG doping efficiency. *Nanoscale Res. Lett.* **2018**, *13*, 122. <https://doi.org/10.1186/s11671-018-2539-9>.
24. Das, S.; Lenka, T.R.; Talukdar, F.A.; Velpula, R.T.; Nguyen, H.P.T. Efficiency and Radiative Recombination Rate Enhancement in GaN/AlGaIn Multi-Quantum Well-Based Electron Blocking Layer Free UV-LED for Improved Luminescence. *FACTA Univ. Ser. Electron. Energ.* **2023**, *36*, 91–101. <https://doi.org/10.2298/FUEE2301091D>.
25. Das, S.; Lenka, T.R.; Talukdar, F.A.; Sadaf, S.M.; Velpula, R.T.; Nguyen, H.P.T. Impact of a pretrained graded InGaIn/GaN interlayer towards enhanced optical characteristics of a multi-quantum well LED based on silicon substrate. *Appl. Opt.* **2022**, *61*, 8951–8958. <https://doi.org/10.1364/AO.470083>.
26. Philip, M.R.; Choudhary, D.D.; Djavid, M.; Le, K.Q.; Piao, J.; Nguyen, H.P.T. High efficiency green/yellow and red InGaIn/AlGaIn nanowire light-emitting diodes grown by molecular beam epitaxy. *J. Sci. Adv. Mater. Devices* **2017**, *2*, 150–155. <https://doi.org/10.1016/j.jsamd.2017.05.009>.
27. Liu, C.; Melanson, B.; Zhang, J. AlgaIn-delta-gan quantum well for duvleds. *Photonics* **2020**, *7*, 87. <https://doi.org/10.3390/photonics7040087>.
28. Das, S.; Lenka, T.R.; Talukdar, F.A.; Nguyen, H.P.T.; Crupi, G. The role of indium composition in  $\text{In}_x\text{Ga}_{1-x}\text{N}$  pretrained layer towards optical characteristics of EBL free GaN/InGaIn nanowire LEDs for enhanced luminescence. *Int. J. Numer. Model.* **2023**, *36*, e3169. <https://doi.org/10.1002/jnm.3169>.
29. Varshni, Y.P. Temperature dependence of the energy gap in semiconductors. *Physica* **1967**, *34*, 149–154.
30. Piprek, J. *Nitride Semiconductor Devices: Principles and Simulation*; Wiley Online Library: Berlin, Germany, 2007; Volume 590.
31. Nunez-Gonzalez, R. First-principles calculation of the band gap of  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  and  $\text{In}_x\text{Ga}_{1-x}\text{N}$ . *Rev. Mex. Fis.* **2008**, *54*, 111–118.
32. Chuang, S.; Chang, C.  $k \cdot p$  method for strained wurtzite semiconductors. *Phys. Rev. B* **1996**, *54*, 2491–2504. <https://doi.org/10.1103/PhysRevB.54.2491>.
33. Caughey, D.M.; Thomas, R.E. Carrier Mobilities in Silicon Empirically Related to Doping and Field. *Proc. IEEE* **1967**, *55*, 2192–2193. <https://doi.org/10.1109/PROC.1967.6123>.
34. Yun, J.; Shim, J.I.; Hirayama, H. Analysis of efficiency droop in 280-nm AlGaIn multiple-quantum-well light-emitting diodes based on carrier rate equation. *Appl. Phys. Express* **2015**, *8*, 022104. <https://doi.org/10.7567/APEX.8.022104>.
35. Hirayama, H. Recent Progress in AlGaIn Deep-UV LEDs. In *Light-Emitting Diode: An Outlook On the Empirical Features and Its Recent Technological Advancements*; BoD—Books on Demand: London, UK, 2018; <https://doi.org/10.5772/intechopen.79936>.
36. Fiorentini, V.; Bernardini, F.; Ambacher, O. Evidence for nonlinear macroscopic polarization in III-V nitride alloy heterostructures. *Appl. Phys. Lett.* **2002**, *80*, 1204–1206. <https://doi.org/10.1063/1.1448668>.

37. Vurgaftman, I.; Meyer, J.R. Band parameters for nitrogen-containing semiconductors. *J. Appl. Phys.* **2003**, *94*, 3675–3696. <https://doi.org/10.1063/1.1600519>.
38. Das, S.; Lenka, T.R.; Talukdar, F.A.; Velpula, R.T.; Nguyen, H.P.T. Design and analysis of novel high-performance III-nitride MQW-based nanowire white-LED using  $\text{HfO}_2/\text{SiO}_2$  encapsulation. *Opt. Quantum Electron.* **2023**, *55*, 67. <https://doi.org/10.1007/s11082-022-04350-y>.
39. Xu, Q.; Niu, Y.; Li, J.; Yang, Z.; Gao, J.; Ding, L.; Ni, H.; Zhu, P.; Liu, Y.; Tang, Y.; et al. Recent progress of quantum dots for energy storage applications. *Carbon Neutrality* **2022**, *1*, 13. <https://doi.org/10.1007/s43979-022-00002-y>.
40. Zhang, Z.H.; Liu, W.; Ju, Z.; Tan, S.T.; Ji, Y.; Kyaw, Z.; Zhang, X.; Wang, L.; Sun, X.W.; Demir, H.V. Self-screening of the quantum confined Stark effect by the polarization induced bulk charges in the quantum barriers. *Appl. Phys. Lett.* **2014**, *104*, 16–21. <https://doi.org/10.1063/1.4883894>.
41. Ambacher, O.; Dimitrov, R.; Stutzmann, M.; Foutz, B.E.; Murphy, M.J.; Smart, J.A.; Shealy, J.R.; Weimann, N.G.; Chu, K.; Chumbes, M.; et al. Role of spontaneous and piezoelectric polarization induced effects in group-III nitride based heterostructures and devices. *Phys. Status Solidi Basic Res.* **1999**, *216*, 381–389. [https://doi.org/10.1002/\(SICI\)1521-3951\(199911\)216:1<381::AID-PSSB381>3.0.CO;2-O](https://doi.org/10.1002/(SICI)1521-3951(199911)216:1<381::AID-PSSB381>3.0.CO;2-O).
42. Kang, Y.; Yu, H.; Ren, Z.; Xing, C.; Liu, Z.; Jia, H.; Guo, W.; Sun, H. Efficiency Droop Suppression and Light Output Power Enhancement of Deep Ultraviolet Light-Emitting Diode by Incorporating Inverted-V-Shaped Quantum Barriers. *IEEE Trans. Electron. Devices* **2020**, *67*, 4958–4962. <https://doi.org/10.1109/TED.2020.3025523>.
43. Jain, B.; Velpula, R.T.; Patel, M.; Sadaf, S.M.; Nguyen, H.P.T. Improved performance of electron blocking layer free algal deep ultraviolet light-emitting diodes using graded staircase barriers. *Micromachines* **2021**, *12*, 334. <https://doi.org/10.3390/mi12030334>.
44. Jain, B.; Velpula, R.T.; Velpula, S.; Nguyen, H.-D.; Nguyen, H.P.T. Enhanced hole transport in AlGaIn deep ultraviolet light-emitting diodes using a double-sided step graded superlattice electron blocking layer. *J. Opt. Soc. Am. B* **2020**, *37*, 2564. <https://doi.org/10.1364/josab.399773>.
45. Ji, Y.; Zhang, Z.H.; Kyaw, Z.; Tan, S.T.; Ju, Z.G.; Zhang, X.L.; Liu, W.; Sun, X.W.; VolkanDemir, H. Influence of n-type versus p-type AlGaIn electron-blocking layer on InGaIn/GaN multiple quantum wells light-emitting diodes. *Appl. Phys. Lett.* **2013**, *103*, 053512. <https://doi.org/10.1063/1.4817381>.
46. Pandey, A.; Shin, W.J.; Liu, X.; Mi, Z. Effect of electron blocking layer on the efficiency of AlGaIn mid-ultraviolet light emitting diodes. *Opt. Express* **2019**, *27*, A738. <https://doi.org/10.1364/oe.27.00a738>.

**Disclaimer/Publisher’s Note:** The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.