

# Correct implementation of polarization constants in wurtzite materials and impact on III-nitrides

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## Supplemental Material

### S1. STRUCTURAL PARAMETERS AND BAND GAPS CALCULATED WITH THE HSE HYBRID FUNCTIONAL

TABLE I. Parameters for the III-nitrides calculated with HSE. Experimental data are listed for comparison.

|     | Property   | HSE (this work) | Experiment <sup>a</sup> |
|-----|------------|-----------------|-------------------------|
| GaN | $a$ (Å)    | 3.205           | 3.189                   |
|     | $c$ (Å)    | 5.200           | 5.185                   |
|     | $u$        | 0.377           | 0.377 <sup>b</sup>      |
|     | $E_g$ (eV) | 3.496           | 3.4-3.5                 |
| AlN | $a$ (Å)    | 3.099           | 3.112                   |
|     | $c$ (Å)    | 4.959           | 4.982                   |
|     | $u$        | 0.382           | 0.382 <sup>b</sup>      |
|     | $E_g$ (eV) | 6.044           | 6.1-6.3                 |
| InN | $a$ (Å)    | 3.587           | 3.545                   |
|     | $c$ (Å)    | 5.762           | 5.703                   |
|     | $u$        | 0.380           | —                       |
|     | $E_g$ (eV) | 0.646           | 0.6-0.8                 |

<sup>a</sup> From Ref. S1 unless otherwise specified.

<sup>b</sup> From Ref. S2.

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## S2. EXPERIMENTAL DETERMINATION OF POLARIZATION FROM THE LITERATURE

The experimental data points in Fig. 2 of the main text were taken from various literature studies that were intended to determine the polarization constants in the InGaN/GaN or AlGaIn/GaN systems. We list these references in Table III, IV, V, and II along with the reported values. Whether the actual measurement was bound charges at an interface or the field in a quantum well, we have converted the reported values to a polarization sheet charge for the purposes of Fig. 2 using the procedure outlined in Sec. V of the main text.

TABLE II. Experimental data for GaN/InGaIn/GaN quantum wells from optical (if not specified), holography, and CV measurements. In the cases where fields are reported in the reference, the bound charge is determined from the model described in the main text, Sec. V.

| Reference        | InGaIn content                                                      | Field ( $10^5$ V/cm)                                                | Bound charge ( $10^{12}e^-/\text{cm}^2$ )                |
|------------------|---------------------------------------------------------------------|---------------------------------------------------------------------|----------------------------------------------------------|
| S3               | 0.08                                                                | 6.0                                                                 | 3.1                                                      |
| S4               | 0.10                                                                | 13.6                                                                | 7.2                                                      |
| S5               | 0.15                                                                | 21.0                                                                | 11.5                                                     |
| S6               | 0.12, 0.22                                                          | 15.0, 29.0                                                          | 8.1, 16.5                                                |
| S7               | 0.10                                                                | 3.5                                                                 | 1.9                                                      |
| S8               | 0.18, 0.15, 0.20                                                    | 24.5, 27.0, 22.0                                                    | 13.6, 14.8, 12.4                                         |
| S9, S10, S11     | 0.07, 0.08, 0.08, 0.08, 0.08, 0.08,<br>0.09, 0.09, 0.09, 0.09, 0.09 | 10.5, 11.4, 11.1, 11.1, 12.6, 12.3,<br>12.9, 13.4, 13.7, 14.0, 14.0 | 5.5, 6.0, 5.8, 5.8, 6.6, 6.5, 6.8, 7.1,<br>7.2, 7.4, 7.4 |
| S12              | 0.07                                                                | 9.3                                                                 | 4.8                                                      |
| S13              | 0.15                                                                | 13.4                                                                | 7.33                                                     |
| S14              | 0.08                                                                | 11.0                                                                | 5.76                                                     |
| S15              | 0.09                                                                | 19.0                                                                | 10.0                                                     |
| S16              | 0.11                                                                |                                                                     | 2.9                                                      |
| S17              | 0.20                                                                | 31.0                                                                | 17.5                                                     |
| S18              | 0.11                                                                | 3.0                                                                 | 1.6                                                      |
| S19              | 0.10                                                                | 9.0                                                                 | 4.8                                                      |
| S20              | 0.14, 0.14, 0.14                                                    | 18.1, 21.2, 20.4                                                    | 9.8, 11.5, 11.1                                          |
| S21              | 0.16                                                                | 12.0                                                                | 6.6                                                      |
| S22              | 0.23                                                                | 18.0                                                                | 10.3                                                     |
| S22 (holography) | 0.18                                                                | 22                                                                  | 12.2                                                     |
| S23 (holography) | 0.52                                                                | 40.0                                                                | 26.8                                                     |
| S24 (holography) | 0.52                                                                | 32.0                                                                | 21.4                                                     |
| S25 (CV)         | 0.08                                                                |                                                                     | 4.1                                                      |
| S26 (CV)         | 0.05, 0.09                                                          |                                                                     | 1.8, 4.4                                                 |

TABLE III. Experimental data for GaN/AlGaN interfaces from Hall-effect measurements.

| Reference | AlGaN content                                                                                                                                     | Bound charge ( $10^{12}e^-/\text{cm}^2$ )                                                                                              |
|-----------|---------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| S27       | 0.09, 0.13, 0.17, 0.26, 0.31, 0.13,<br>0.18, 0.22, 0.22, 0.26, 0.29, 0.29,<br>0.31                                                                | 3.9, 4.9, 8.7, 13.8, 15.0, 6.8, 7.2,<br>8.2, 11.0, 10.2, 10.1, 13.4, 13.5                                                              |
| S28       | 0.20, 0.20, 0.30, 0.35, 0.40, 0.40,<br>0.40, 0.40, 0.40, 0.37                                                                                     | 9.8, 15.1, 19.1, 23.6, 28.5, 25.4,<br>24.1, 22.0, 19.7, 20.1                                                                           |
| S29       | 0.33, 0.34, 0.38                                                                                                                                  | 13.2, 9.0, 10.5                                                                                                                        |
| S30       | 0.15                                                                                                                                              | 6.0                                                                                                                                    |
| S31       | 0.15                                                                                                                                              | 7.9                                                                                                                                    |
| S32       | 0.3 0                                                                                                                                             | 16.0                                                                                                                                   |
| S33       | 0.05, 0.15                                                                                                                                        | 2.3, 6.7                                                                                                                               |
| S34       | 0.02, 0.06, 0.09, 0.14, 0.02, 0.05,<br>0.13, 0.15, 0.19, 0.24, 0.29                                                                               | 1.1, 2.1, 3.0, 3.3, 1.2, 1.6, 4.4, 4.6,<br>5.6, 6.5, 8.0                                                                               |
| S35       | 0.12, 0.14, 0.14, 0.17, 0.17, 0.20,<br>0.23, 0.24, 0.26, 0.30, 0.31, 0.34,<br>0.36, 0.37                                                          | 3.5, 4.6, 4.3, 5.6, 5.6, 6.5, 7.9, 8.8,<br>9.1, 10.7, 11.6, 12.3, 12.6, 14.0                                                           |
| S36       | 0.23                                                                                                                                              | 11.0                                                                                                                                   |
| S37       | 0.16                                                                                                                                              | 7.3                                                                                                                                    |
| S38       | 0.10, 0.13, 0.18                                                                                                                                  | 2.8, 4.1, 6.2                                                                                                                          |
| S39       | 0.10, 0.15, 0.20                                                                                                                                  | 4.1, 6.3, 8.7                                                                                                                          |
| S40       | 0.13, 0.23, 0.26, 0.36                                                                                                                            | 7.3, 9.5, 11.0, 15.2                                                                                                                   |
| S41       | 0.22, 0.26, 0.32, 0.36                                                                                                                            | 7.3, 9.0, 11.3, 12.0                                                                                                                   |
| S42       | 1.0                                                                                                                                               | 34                                                                                                                                     |
| S43       | 0.20                                                                                                                                              | 13                                                                                                                                     |
| S44       | 0.05, 0.15, 0.15, 0.15, 0.25, 0.35                                                                                                                | 3.0, 8.0, 7.5, 5.9, 9.9, 18.0                                                                                                          |
| S45       | 0.23                                                                                                                                              | 9.8                                                                                                                                    |
| S46       | 0.06, 0.10, 0.26, 0.33                                                                                                                            | 1.0, 1.9, 1.4, 1.8                                                                                                                     |
| S47       | 0.72                                                                                                                                              | 35                                                                                                                                     |
| S48       | 0.21, 0.21, 0.27, 0.33, 0.33, 0.40,<br>0.40, 0.49, 0.48                                                                                           | 9.2, 10.1, 11.0, 11.5, 11.2, 12.9,<br>13.3, 16.9, 16.4                                                                                 |
| S49       | 0.15, 0.19, 0.18, 0.19, 0.20, 0.20,<br>0.23, 0.22, 0.26, 0.27, 0.26, 0.31,<br>0.31, 0.32, 0.32, 0.34, 0.35, 0.37,<br>0.37, 0.36, 0.43, 0.44, 0.46 | 0.7, 1.1, 1.4, 2.8, 3.0, 6.9, 6.4, 4.8,<br>11.2, 11.0, 8.7, 12.2, 13.0, 14.1, 9.8,<br>11.0, 9.6, 10.1, 11.4, 14.7, 13.6,<br>14.0, 14.3 |
| S50       | 0.26                                                                                                                                              | 25                                                                                                                                     |

TABLE IV. Experimental data for AlGaIn/GaN/AlGaIn quantum wells from optical and holography measurements. In the cases where fields are reported in the reference, the bound charge is determined from the model described in the main text, Sec. V.

| Reference        | AlGaIn content                                       | Field ( $10^5$ V/cm)                                | Bound charge ( $10^{12}e^-/\text{cm}^2$ )   |
|------------------|------------------------------------------------------|-----------------------------------------------------|---------------------------------------------|
| S51              | 0.08, 0.08, 0.13, 0.17, 0.13, 0.17, 0.27, 0.27       |                                                     | 3.8, 3.0, 5.6, 7.2, 7.4, 9.4, 14.2, 10.9    |
| S52              | 0.15                                                 |                                                     | 2.0                                         |
| S53              | 0.50                                                 | 42.7                                                | 21.2                                        |
| S54              | 0.20, 0.20                                           | 12.8, 8.3                                           | 6.4, 4.1                                    |
| S54 (Holography) | 0.20, 0.20, 0.20                                     | 12.8, 8.4, 6.9                                      | 6.4, 4.2, 3.4                               |
| S55              | 0.24                                                 | 15.0                                                | 7.5                                         |
| S56              | 0.17                                                 | 8.3                                                 | 4.1                                         |
| S57              | 0.65                                                 | 20                                                  | 9.94                                        |
| S58, S59         | 0.07                                                 | 4.8                                                 | 2.4                                         |
| S60              | 0.14                                                 | 5.1                                                 | 2.5                                         |
| S61              | 0.18, 0.11, 0.15                                     | 10.2, 9.3, 3.8                                      | 5.1, 4.6, 1.9                               |
| S62              | 0.18                                                 | 12.3                                                | 6.1                                         |
| S63              | 0.20, 0.50, 0.65, 0.80                               | 11.9, 29.5, 33.9, 49.2                              | 5.9, 14.6, 16.8, 24.5                       |
| S64              | 0.15                                                 | 3.5                                                 | 1.74                                        |
| S56              | 0.11                                                 | 4.5                                                 | 2.24                                        |
| S65              | 0.24, 0.18, 0.18, 0.15, 0.07, 0.18, 0.17, 0.16, 0.16 | 13.0, 13.0, 13.2, 9.0, 4.1, 13.3, 10.0, 10.0, 10.2  |                                             |
| S66              | 0.07, 0.15, 0.17, 0.18, 0.24, 0.18, 0.16, 0.16, 0.17 | 5.3, 11.7, 17.2, 16.9, 19.5, 13.8, 10.6, 10.2, 10.1 | 2.6, 5.8, 8.5, 8.4, 9.7, 6.9, 5.3, 5.1, 5.0 |
| S67              | 0.15                                                 | 14                                                  | 7.0                                         |
| S45              | 0.23                                                 |                                                     | 10.2                                        |
| S46              | 0.06, 0.10, 0.26, 0.33                               | 3.4, 3.1, 3.8, 3.4                                  | 1.7, 1.5, 1.9, 1.7                          |
| S68              | 0.31                                                 |                                                     | 11.0                                        |
| S69              |                                                      |                                                     |                                             |
| S70              | 0.19                                                 | 2.5                                                 | 7.4                                         |

TABLE V. Experimental data for GaN/AlGaIn interfaces from CV measurements.

| Reference | AlGaIn content               | Bound charge ( $10^{12}e^-/\text{cm}^2$ ) |
|-----------|------------------------------|-------------------------------------------|
| S71       | 0.22                         | 1.3                                       |
| S72       | 0.15                         | 3.8                                       |
| S49       | 0.33                         | 10, 12                                    |
| S73       | 0.09, 0.13, 0.17, 0.26, 0.31 | 3.8, 4.9, 8.7, 13.6, 15.0                 |
| S74       | 0.05, 0.12, 0.16             | 2.3, 6.8, 6.9                             |
| S25       | 0.13                         | 7.1                                       |
| S34       | 0.02, 0.06, 0.09, 0.14       | 0.9, 1.8, 2.0, 3.1                        |
| S50       | 0.26                         | 7.0                                       |

### S3. BOUND CHARGES AT NITRIDE INTERFACES

Here we present the specific equations used to generate Fig. 2 in the main text. As in the main text, we assume a coherent  $c$  plane interface of GaN and the alloy (InGa<sub>*N*</sub> or AlGa<sub>*N*</sub>), with the alloy layer under biaxial stress. The current practice in the field (black dashed curve in Fig. 2 of the main text) is to use the effective spontaneous (SP) polarization constants with respect to the zincblende (ZB) reference, without the correction term [ $\Delta P_{\text{corr}}^{\text{ref}}$  introduced in Eq. (11) of the main text], and the proper piezoelectric (PZ) constants. (These values are usually taken from Ref. S75.) The resulting equation for Al<sub>*x*</sub>Ga<sub>1-*x*</sub>N/GaN is

$$\sigma_{\text{b}}^{(\text{ZB ref}), \text{prop}}(x) = \Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{ZB ref})} x - 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left\{ e_{31}^{\text{AlN}, \text{prop}} x + e_{31}^{\text{GaN}, \text{prop}} (1-x) \right. \\ \left. - [e_{33}^{\text{AlN}, \text{prop}} x + e_{33}^{\text{GaN}, \text{prop}} (1-x)] \frac{C_{13}^{\text{AlN}} x + C_{13}^{\text{GaN}} (1-x)}{C_{33}^{\text{AlN}} x + C_{33}^{\text{GaN}} (1-x)} \right\}, \quad (1)$$

where  $\Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{ZB ref})}$  is

$$\Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{ZB ref})} = P_{\text{eff}}^{\text{GaN}, (\text{ZB ref})} - P_{\text{eff}}^{\text{AlN}, (\text{ZB ref})}. \quad (2)$$

An identical set of equations are used for In<sub>*x*</sub>Ga<sub>1-*x*</sub>N/GaN, with InN instead of AlN.

The red solid curve in Fig. 2 corresponds to using the H ref (or ZB with the correction term) and the improper PZ constants:

$$\sigma_{\text{b}}^{(\text{H ref}), \text{imp}}(x) = \Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{H ref})} x - 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left\{ \left( e_{31}^{\text{AlN}, \text{prop}} - P_{\text{eff}}^{\text{AlN}, (\text{H ref})} \right) x \right. \\ \left. + \left( e_{31}^{\text{GaN}, \text{prop}} - P_{\text{eff}}^{\text{GaN}, (\text{H ref})} \right) (1-x) - [e_{33}^{\text{AlN}, \text{prop}} x + e_{33}^{\text{GaN}, \text{prop}} (1-x)] \frac{C_{13}^{\text{AlN}} x + C_{13}^{\text{GaN}} (1-x)}{C_{33}^{\text{AlN}} x + C_{33}^{\text{GaN}} (1-x)} \right\} \\ = (\Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{ZB ref})} + \Delta P_{\text{corr}}^{(\text{ZB ref})}) x - 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left\{ \left( e_{31}^{\text{AlN}, \text{prop}} - P_{\text{eff}}^{\text{AlN}, (\text{H ref})} \right) x \right. \\ \left. + \left( e_{31}^{\text{GaN}, \text{prop}} - P_{\text{eff}}^{\text{GaN}, (\text{H ref})} \right) (1-x) - [e_{33}^{\text{AlN}, \text{prop}} x + e_{33}^{\text{GaN}, \text{prop}} (1-x)] \frac{C_{13}^{\text{AlN}} x + C_{13}^{\text{GaN}} (1-x)}{C_{33}^{\text{AlN}} x + C_{33}^{\text{GaN}} (1-x)} \right\}, \quad (3)$$

where

$$\Delta P_{\text{corr}}^{(\text{ZB ref})} = \frac{e\sqrt{3}}{2} \left( \frac{1}{(a_{\text{GaN}})^2} - \frac{1}{(a_{\text{AlN}})^2} \right), \quad (4)$$

and similarly for InGa<sub>*N*</sub>/GaN.

#### S4. DIFFERENCE BETWEEN IMPLEMENTATIONS

The difference between the current practice in the field (ZB reference, no correction term, proper PZ) and our revised implementation (H reference, improper PZ constants) can be determined by taking the difference of Eq. (1) and Eq. (3). For the case of AlGaIn/GaN:

$$\begin{aligned}
\sigma_b^{(\text{H ref}), \text{imp}}(x) - \sigma_b^{(\text{ZB ref}), \text{prop}}(x) &= x \left[ \Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{H ref})} - \Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{ZB ref})} \right] \\
&\quad - 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left[ -P_{\text{eff}}^{\text{AlN}, (\text{H ref})}(x) - P_{\text{eff}}^{\text{GaN}, (\text{H ref})}(1-x) \right] \\
&= x \left[ \left( \Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{ZB ref})} + \Delta P_{\text{corr}}^{(\text{ZB ref})} \right) - \Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{ZB ref})} \right] \\
&\quad + 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left[ P_{\text{eff}}^{\text{AlN}, (\text{H ref})}(x) + P_{\text{eff}}^{\text{GaN}, (\text{H ref})}(1-x) \right] \\
&= x \Delta P_{\text{corr}}^{(\text{ZB ref})} + 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left[ P_{\text{eff}}^{\text{AlN}, (\text{H ref})}(x) + P_{\text{eff}}^{\text{GaN}, (\text{H ref})}(1-x) \right] \\
&= x \Delta P_{\text{corr}}^{(\text{ZB ref})} + 2\varepsilon_1(x) P_{\text{eff}}^{\text{AlGaIn}, (\text{H ref})}(x).
\end{aligned} \tag{5}$$

We can gain some more insight by linearizing the first term in Eq. (5):

$$\begin{aligned}
x \Delta P_{\text{corr}}^{(\text{ZB ref})} &= x \frac{e\sqrt{3}}{2} \left( \frac{1}{(a_{\text{GaN}})^2} - \frac{1}{(a_{\text{AlN}})^2} \right) \\
&= x \frac{e\sqrt{3}}{2} \frac{1}{(a_{\text{GaN}})^2} \left( 1 - \frac{(a_{\text{GaN}})^2}{(a_{\text{AlN}})^2} \right) \\
&= x P_{\text{f}}^{\text{GaN}, \text{ZB}} \left( 1 - \frac{(a_{\text{GaN}})^2}{(a_{\text{AlN}})^2} \right) \\
&\simeq 2x P_{\text{f}}^{\text{GaN}, \text{ZB}} \left( 1 - \frac{a_{\text{GaN}}}{a_{\text{AlN}}} \right) \\
&= -2P_{\text{f}}^{\text{GaN}, \text{ZB}} \left( x \frac{a_{\text{GaN}} - a_{\text{AlN}}}{a_{\text{AlN}}} \right) \\
&\simeq -2P_{\text{f}}^{\text{GaN}, \text{ZB}} \varepsilon_1(x)
\end{aligned} \tag{6}$$

So we see that the difference in implementations is

$$\begin{aligned}
\sigma_b^{(\text{H ref}), \text{imp}}(x) - \sigma_b^{(\text{ZB ref}), \text{prop}}(x) &\simeq 2\varepsilon_1(x) \left[ P_{\text{eff}}^{\text{AlGaIn}, (\text{H ref})}(x) - P_{\text{f}}^{\text{GaN}, \text{ZB}} \right] \\
&= 2\varepsilon_1(x) \left[ x P_{\text{f}}^{\text{AlN}, \text{WZ}} + (1-x) P_{\text{f}}^{\text{GaN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{ZB}} \right] \\
&= 2\varepsilon_1(x) \left[ x \left( P_{\text{f}}^{\text{AlN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{WZ}} \right) + \left( P_{\text{f}}^{\text{GaN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{ZB}} \right) \right] \\
&= 2\varepsilon_1(x) \left[ x \left( P_{\text{f}}^{\text{AlN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{WZ}} \right) + P_{\text{eff}}^{\text{GaN}, (\text{ZB ref})} \right]
\end{aligned} \tag{7}$$

Therefore, the difference is small for small strains, and/or when there is a large cancellation of the terms in the square brackets. We see from Table I of the main text that  $P_{\text{f}}^{\text{AlN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{WZ}} = 0.039 \text{ C/m}^2 \sim -P_{\text{eff}}^{\text{GaN}, (\text{ZB ref})}$ , hence the close agreement with between the black dashed and red solid curves in Fig. 2(b) of the main text (along with the relatively small magnitude of the strain). For the case of InGaIn,  $P_{\text{f}}^{\text{InN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{WZ}} = -0.286 \text{ C/m}^2$  which is the same sign as  $P_{\text{eff}}^{\text{GaN}, (\text{ZB ref})}$ , hence the larger discrepancy between the black dashed and red solid curves in Fig. 2(a) of the main text (also combined with a larger strain between InN and GaN).

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