

# Valence band engineering and light emission polarization in deep UV LED

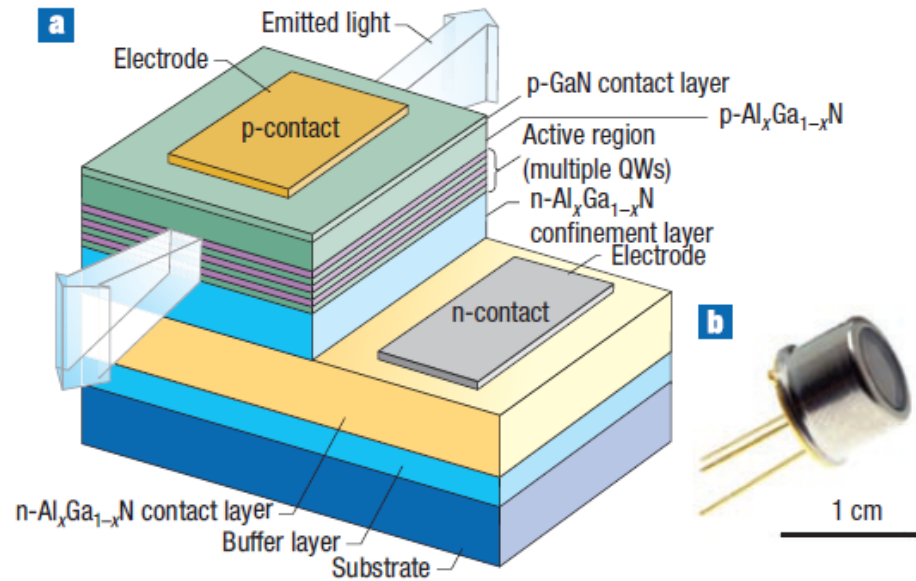
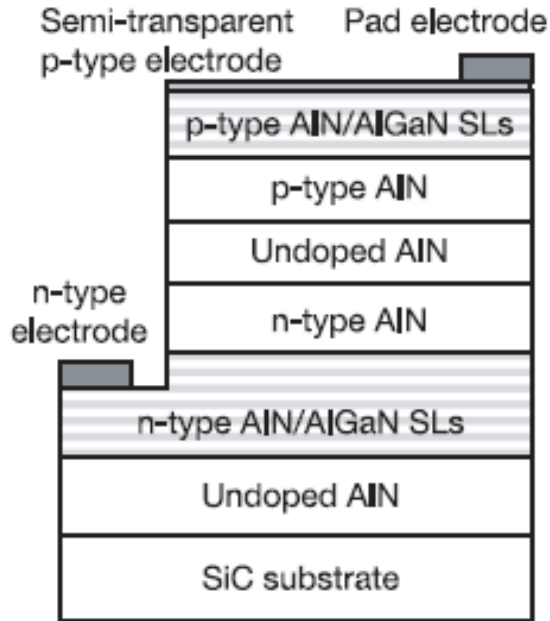
Boxiu Cai, Ronghua Wang, Wenjie Chen

Nov. 2009

# Outline

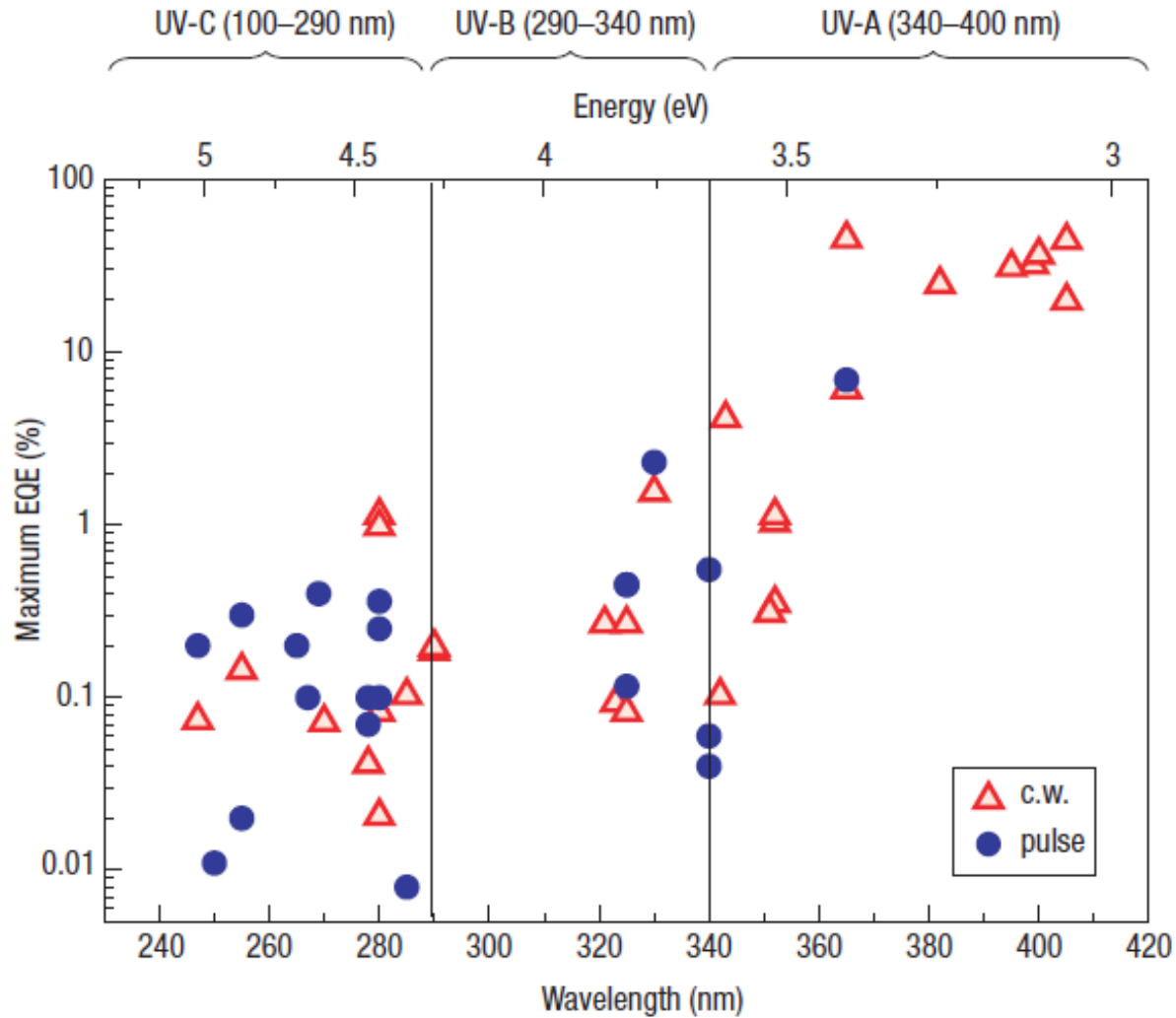
- Introduction to DUV LED;
- Main focus: band structure and polarization;
- Calculation of band structure for unstrained  $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ;
- Calculation of quantum confined  $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ;
- Light emission polarization for bulk  $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ;

# Introduction

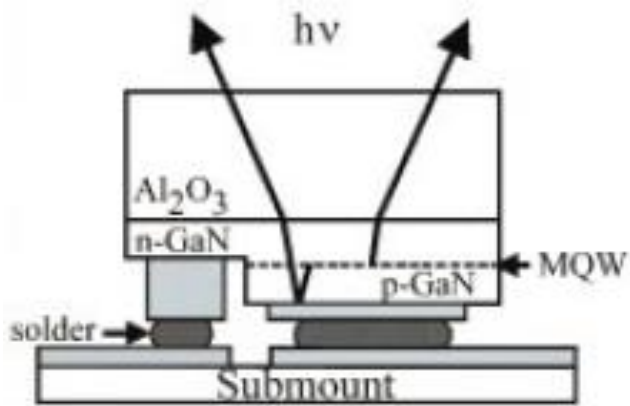


Taniyasu, Y., Kasu, M. and Makimoto, T. An aluminium nitride light-emitting diode with a wavelength of 210 nanometres. *Nature* 441, 325–328 (2006)

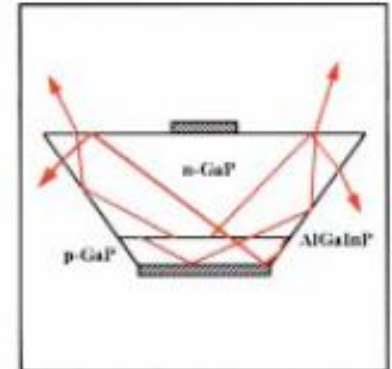
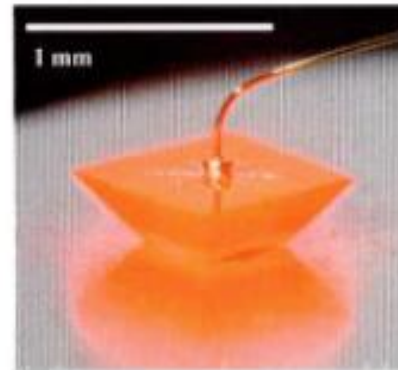
Asif K., Krishnan B. and Tom Kat ona. Ultraviolet light-emitting diodes based on group three nitrides. *Nature photonics*, VOL 2, 2008



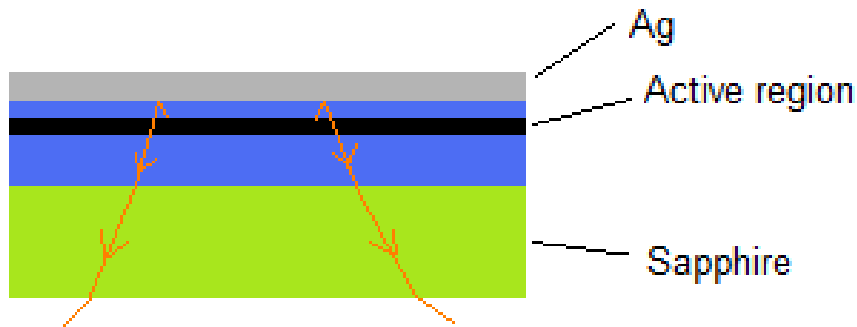
Asif K., Krishnan B. and Tom Kat ona. Ultraviolet light-emitting diodes based on group three nitrides. Nature photonics, VOL 2, 2008



Lumileds Flip-Chip LED



Lumileds truncated-inverted-pyramid LED



conventional LED with a planar Ag reflector

# Main focus

- Band structure calculation for AlGa<sub>x</sub>N at different Al fraction
- Polarization for different band structure
- Quantum confined AlGa<sub>x</sub>N

# Unstrained band structure calculation

Basis set

Kane model :  $8 \times 8$   $k \cdot p$

$$H_{8 \times 8} = \frac{\hbar^2 k^2}{2m_0} + \begin{bmatrix} E_c & -\frac{k_+ P_2}{\sqrt{2}} & \frac{k_- P_2}{\sqrt{2}} & k_z P_1 & 0 & 0 & 0 & 0 \\ -\frac{k_- P_2}{\sqrt{2}} & E_v + \Delta_1 + \Delta_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{k_+ P_2}{\sqrt{2}} & 0 & E_v + \Delta_1 - \Delta_2 & 0 & 0 & 0 & 0 & \sqrt{2} \Delta_3 \\ k_z P_1 & 0 & 0 & E_v & 0 & 0 & \sqrt{2} \Delta_3 & 0 \\ 0 & 0 & 0 & 0 & E_c & \frac{k_- P_2}{\sqrt{2}} & -\frac{k_+ P_2}{\sqrt{2}} & k_z P_1 \\ 0 & 0 & 0 & 0 & \frac{k_+ P_2}{\sqrt{2}} & E_v + \Delta_1 + \Delta_2 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2} \Delta_3 & -\frac{k_- P_2}{\sqrt{2}} & 0 & E_v + \Delta_1 - \Delta_2 & 0 \\ 0 & 0 & \sqrt{2} \Delta_3 & 0 & k_z P_1 & 0 & 0 & E_v \end{bmatrix}$$

$|iS\uparrow\rangle$   
 $u_1 = \left| -\frac{(X+iY)}{\sqrt{2}} \uparrow \right\rangle$   
 $u_2 = \left| \frac{(X-iY)}{\sqrt{2}} \uparrow \right\rangle$   
 $u_3 = |Z\uparrow\rangle$   
 $|iS\downarrow\rangle$   
 $u_4 = \left| \frac{(X-iY)}{\sqrt{2}} \downarrow \right\rangle$   
 $u_5 = \left| -\frac{(X+iY)}{\sqrt{2}} \downarrow \right\rangle$   
 $u_6 = |Z\downarrow\rangle$

# Momentum-matrix elements

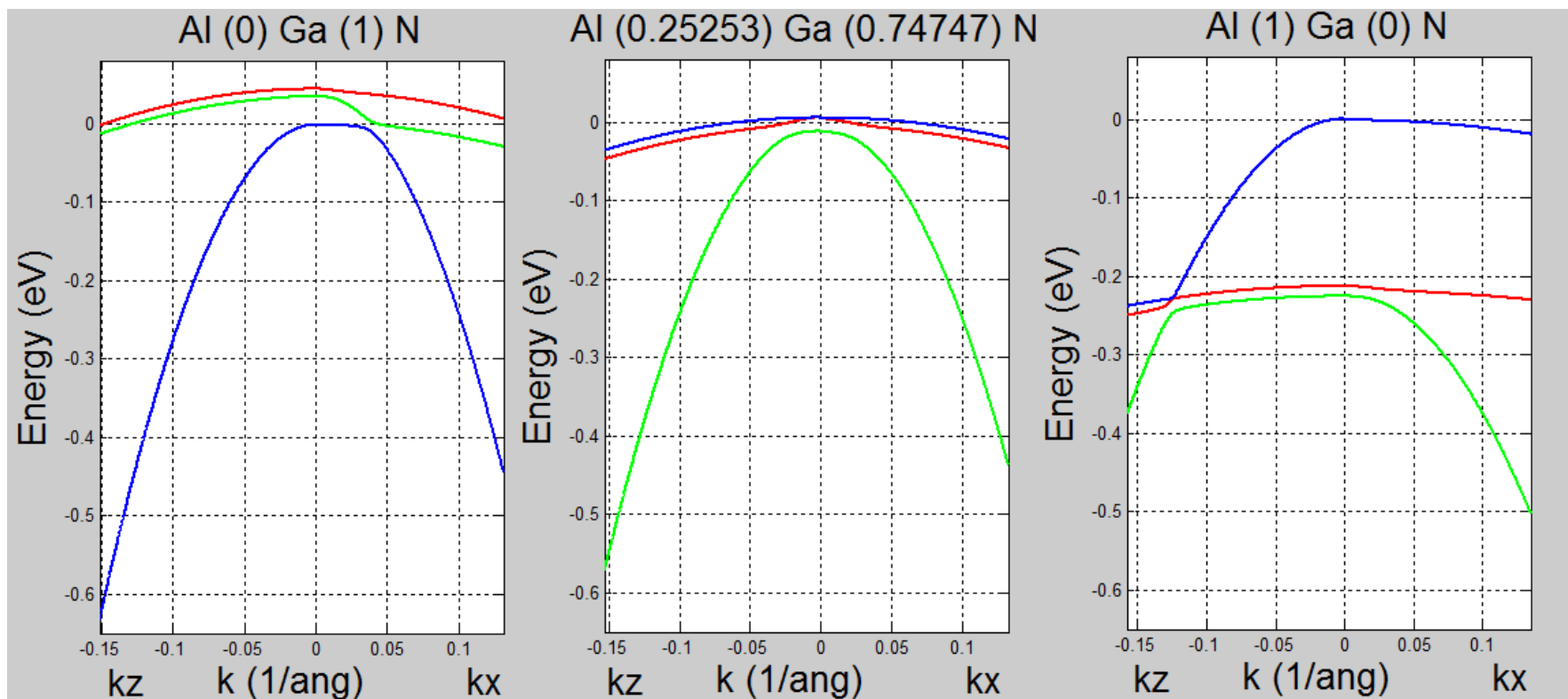
$$\left\langle iS \left| \frac{\hbar}{i} \frac{\partial}{\partial z} \right| Z \right\rangle = \frac{m_0}{\hbar} P_1,$$

$$\left\langle iS \left| \frac{\hbar}{i} \frac{\partial}{\partial x} \right| X \right\rangle = \left\langle iS \left| \frac{\hbar}{i} \frac{\partial}{\partial y} \right| Y \right\rangle = \frac{m_0}{\hbar} P_2.$$

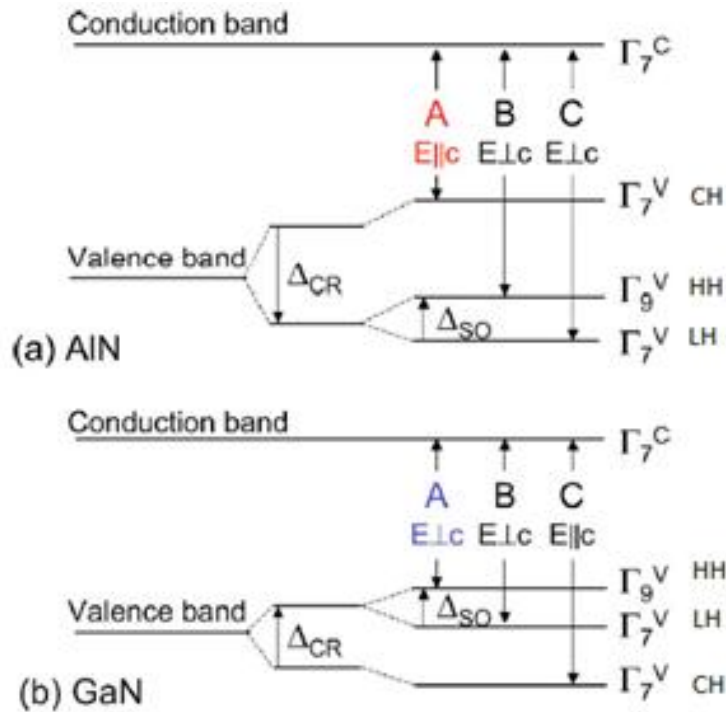
$$P_1^2 = \frac{\hbar^2}{2m_0} \left( \frac{m_0}{m_e^z} - 1 \right) \frac{(E_g + \Delta_1 + \Delta_2)(E_g + 2\Delta_2) - 2\Delta_3^2}{(E_g + 2\Delta_2)},$$

$$P_2^2 = \frac{\hbar^2}{2m_0} \left( \frac{m_0}{m_e^t} - 1 \right) \frac{E_g[(E_g + \Delta_1 + \Delta_2)(E_g + 2\Delta_2) - 2\Delta_3^2]}{(E_g + \Delta_1 + \Delta_2)(E_g + \Delta_2) - \Delta_3^2}, \quad (18)$$

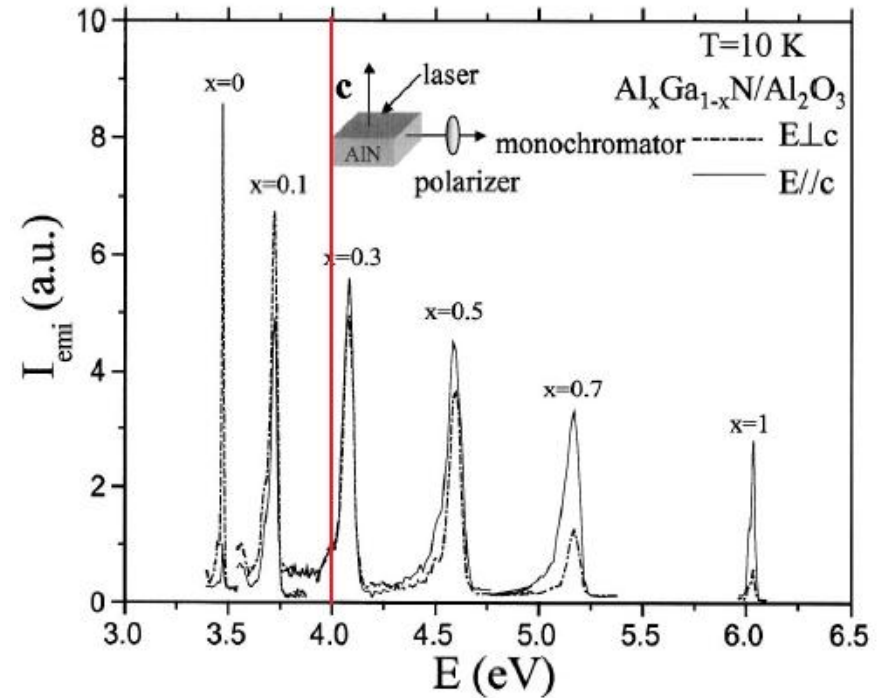
# Band structure changing trend with Al composition



# Light Emission Polarization



*APL, 90, 261911 (2007)*



*APL, 84, 5264 (2004)*

# C-CH transition in bulk AlGaN ( $x > 0.25$ )

Momentum-matrix elements

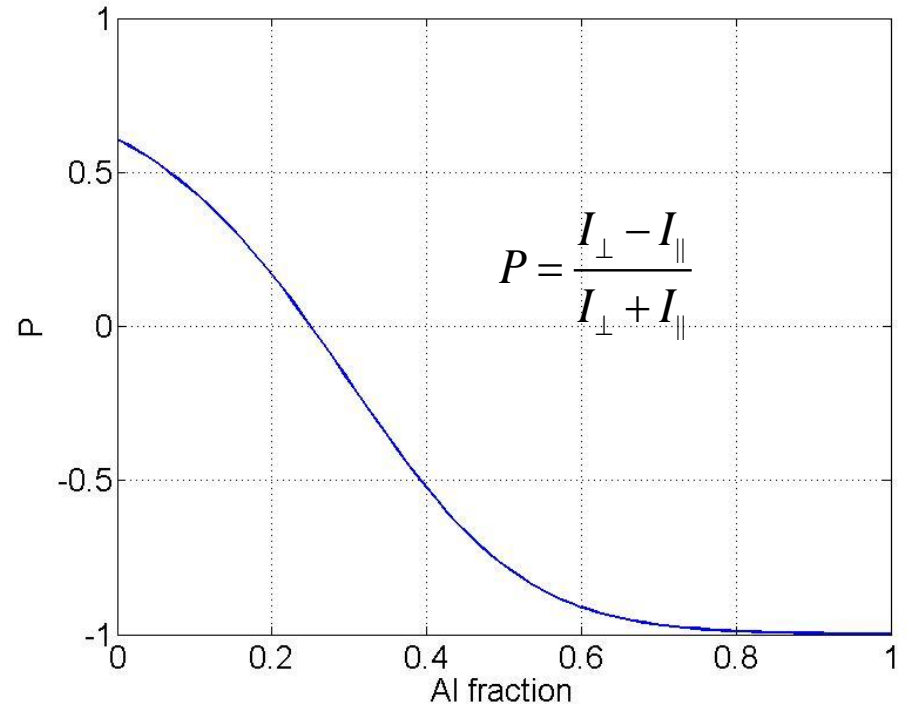
$$|\langle S | \hat{e} \cdot \mathbf{p} | V \rangle|^2$$

Wave function symmetric :

S X, Y, Z  
 HH X, Y  
 LH X, Y dominant  
 CH Z dominant

Valence energy	$\hat{e}_{\parallel} c$ axis	$\hat{e}_{\perp} c$ axis
$E_1$ (CH band)	$b^2 \left( \frac{m_0}{2} E_{pz} \right)$	$a^2 \left( \frac{m_0}{4} E_{px} \right)$
$E_2$ (HH band)	0	$\frac{m_0}{4} E_{px}$
$E_3$ (LH band)	$a^2 \left( \frac{m_0}{2} E_{pz} \right)$	$b^2 \left( \frac{m_0}{4} E_{px} \right)$
Sum	$\frac{m_0}{2} E_{pz}$	$\frac{m_0}{2} E_{px}$

The degree of polarization ( $P$ )

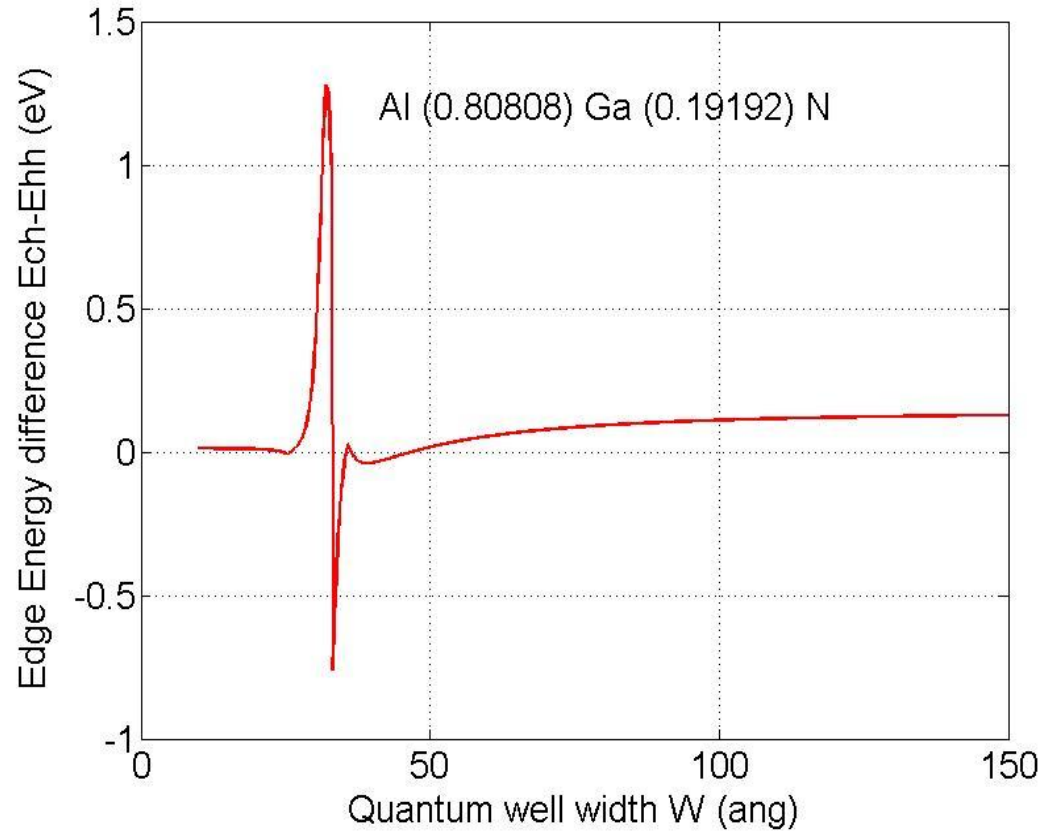


$$I_{\perp} = a^2 \left( \frac{m_0}{4} E_{px} \right) = \frac{E_2^2}{E_2^2 + 2\Delta_3^2} \cdot \frac{m_0^2}{2\hbar^2} P_2^2$$

$$I_{\parallel} = b^2 \left( \frac{m_0}{2} E_{pz} \right) = \frac{2\Delta_3^2}{E_2^2 + 2\Delta_3^2} \cdot \frac{m_0^2}{\hbar^2} P_1^2$$

*Physical Review B*, 54, 2491 (1996)

# Quantum Confinement



# Future Work

- Calculation of the band structures and polarization degree for strained  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  band structures;
- Light emission polarization switch by quantum confinement for strained  $\text{Al}_x\text{Ga}_{1-x}\text{N}$ .