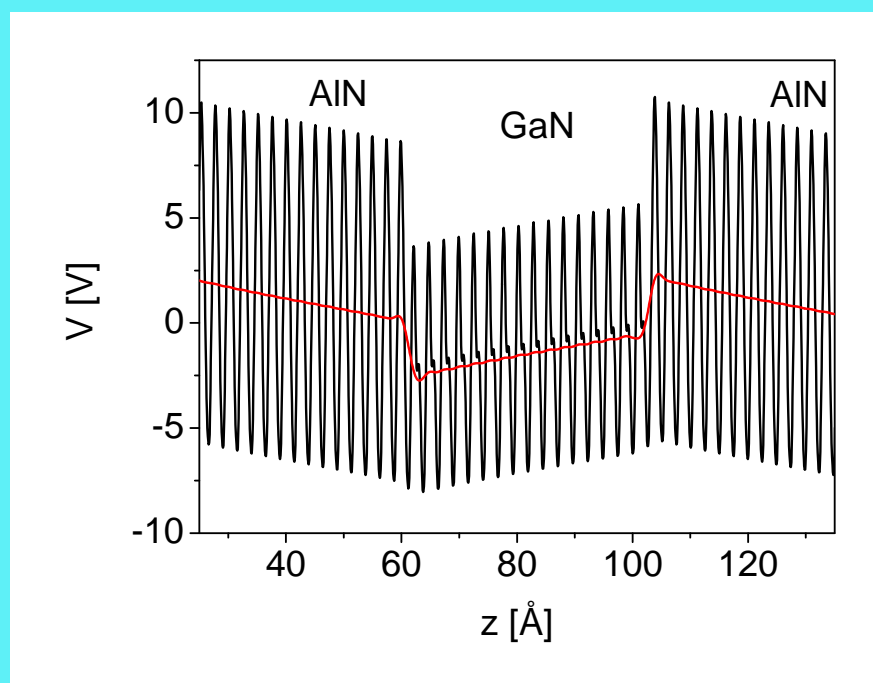


Polarization, polarization doping and multiquantum wells

P. Strak, P. Kempisty, K. Sakowski, A. Ahmad, Z. Romanowski, S. Krukowski, A. Kamińska, E. Grzanka, M. Leszczyński, M. Sarzyński, G. Muzioł, I. Grzegory

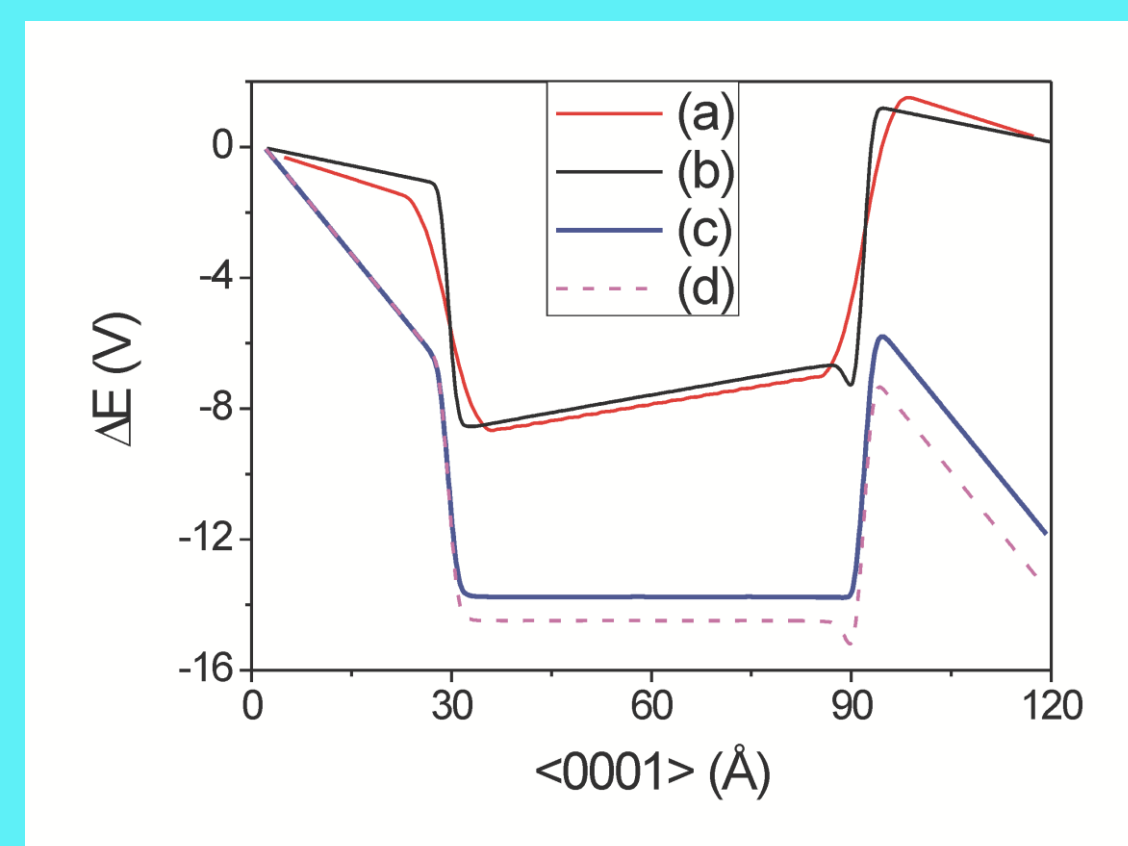
New methodology – *ab initio* calculations (SIESTA & VASP)

Potential averaging



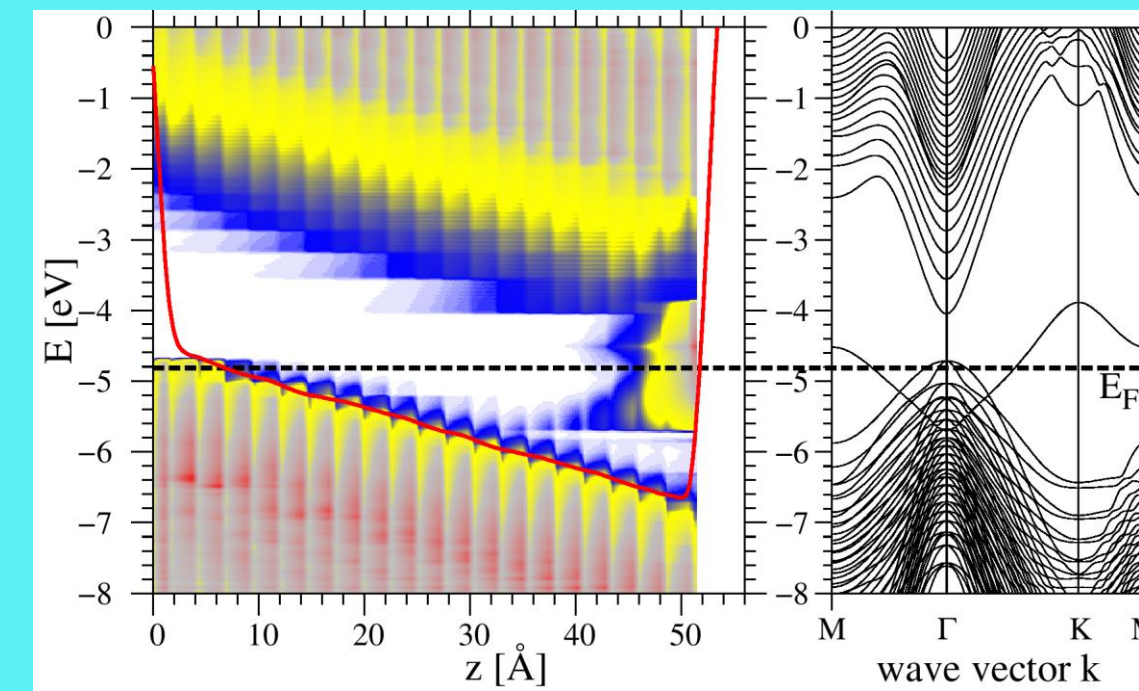
- In-plane and c-axis adjacent averaging
- Smoothed potential profiles
- Charges & dipoles are obtained

Compensating field in empty space



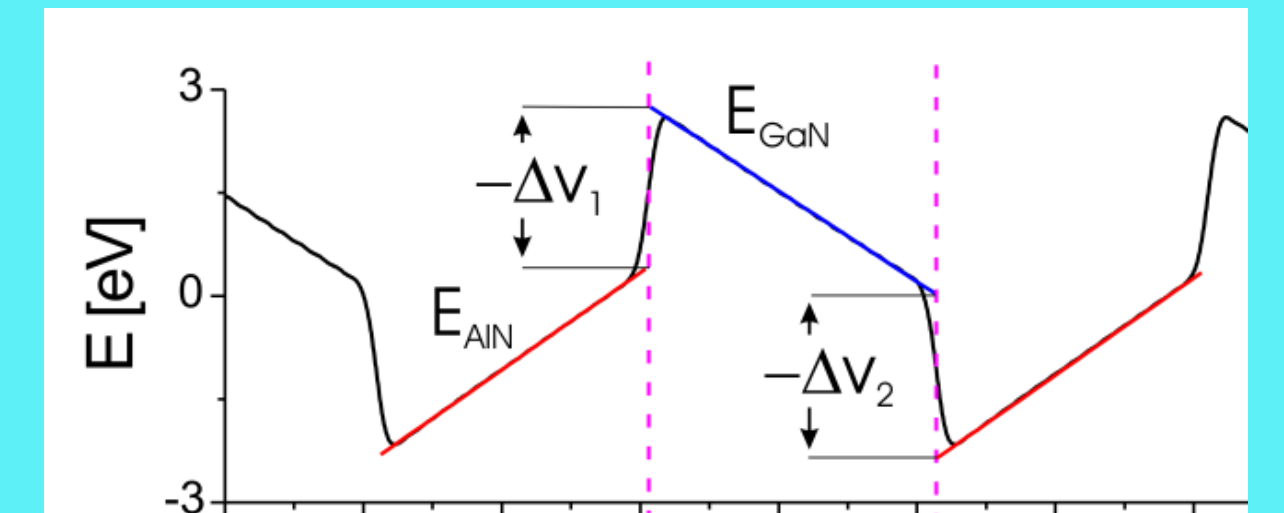
$$P_{slab}^{(pol)} = \frac{P_{slab}^{(0)}}{\epsilon} \quad E_{slab}^{(pol)} = -\frac{P_{slab}^{(0)}}{\epsilon \epsilon_0}$$

Real space band visualization



- Fields in the slabs
- Charge in the system

Charges & dipoles – potential slope and value jumps

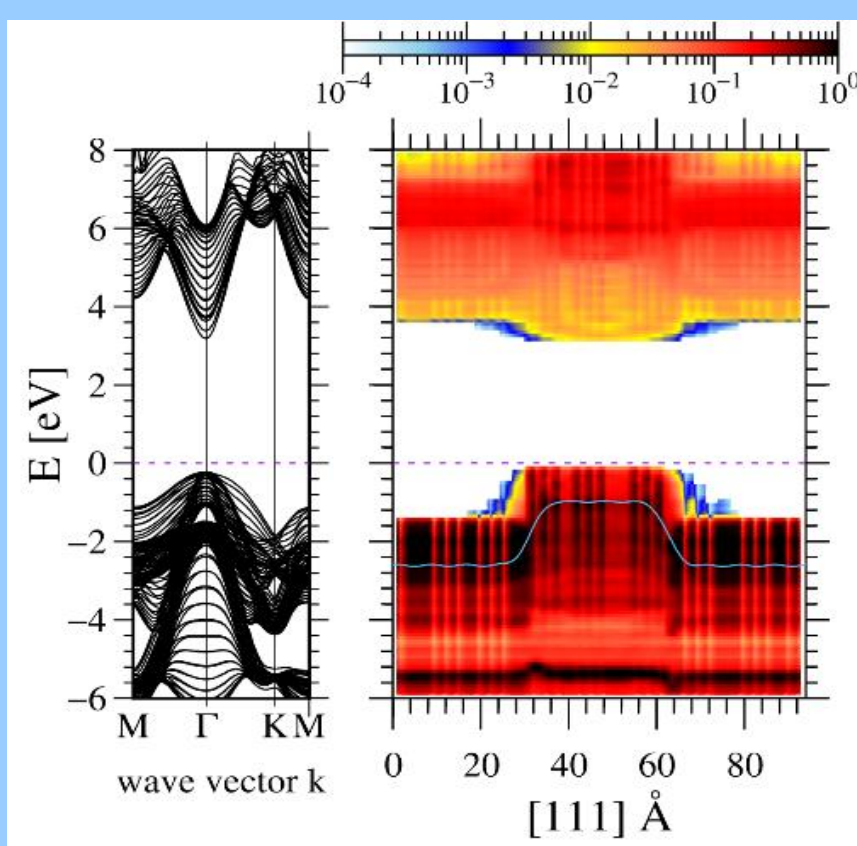


- Interface charge density
- Dipole moment density

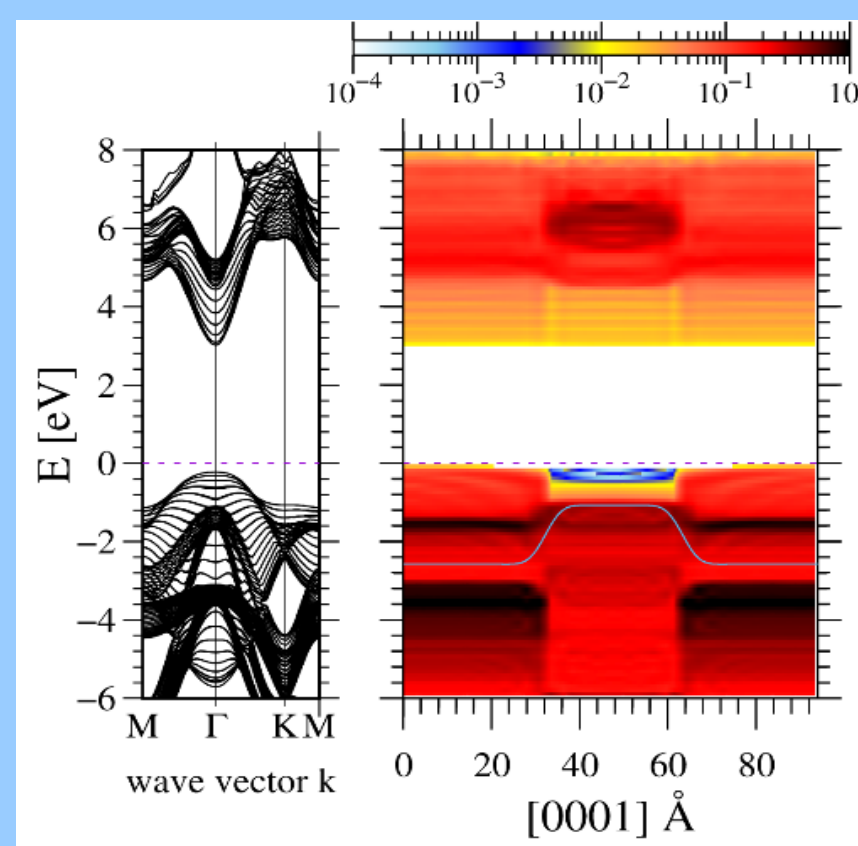
Polarization – Quantum Confined Stark Effect (QCSE)

Spontaneous polarization & piezo effects 24 AIN-12GaN supercell

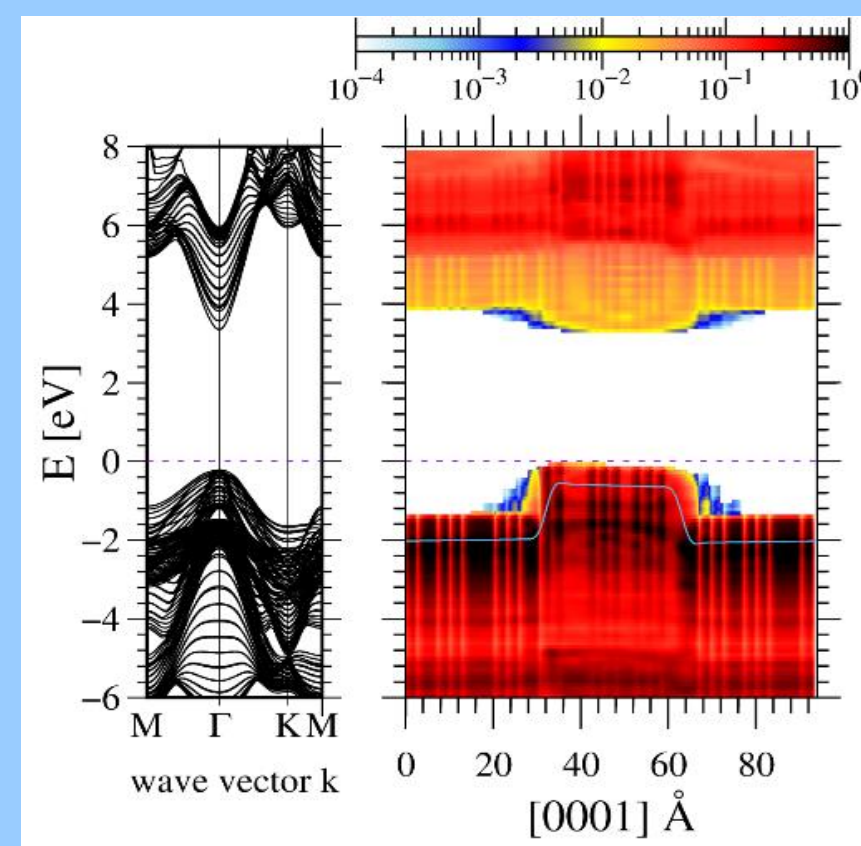
Zinc blende



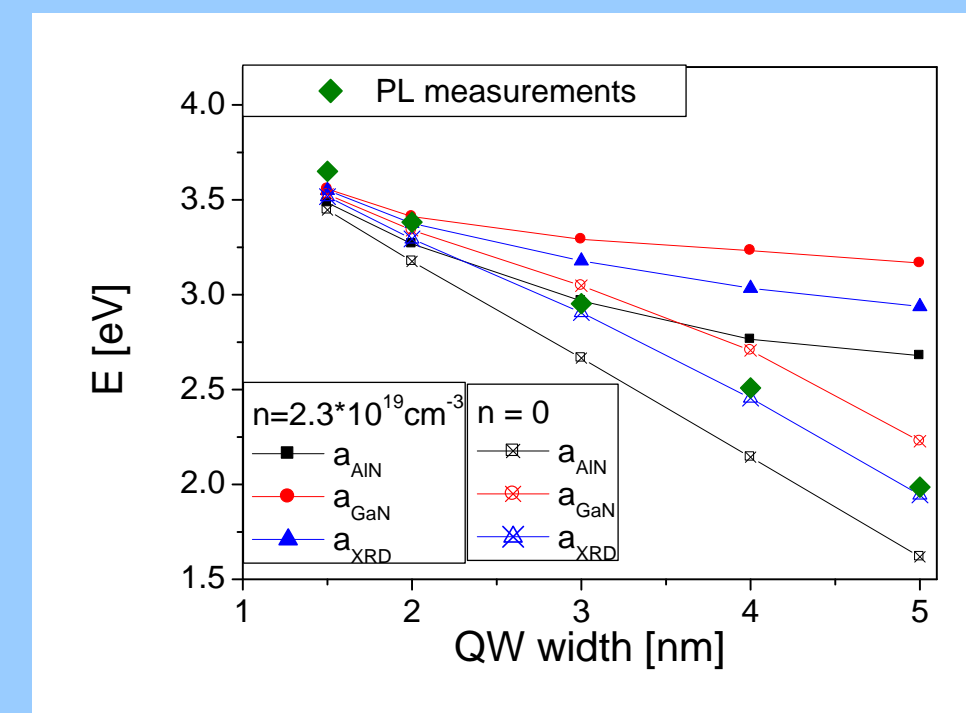
Hexagonal



Wurtzite

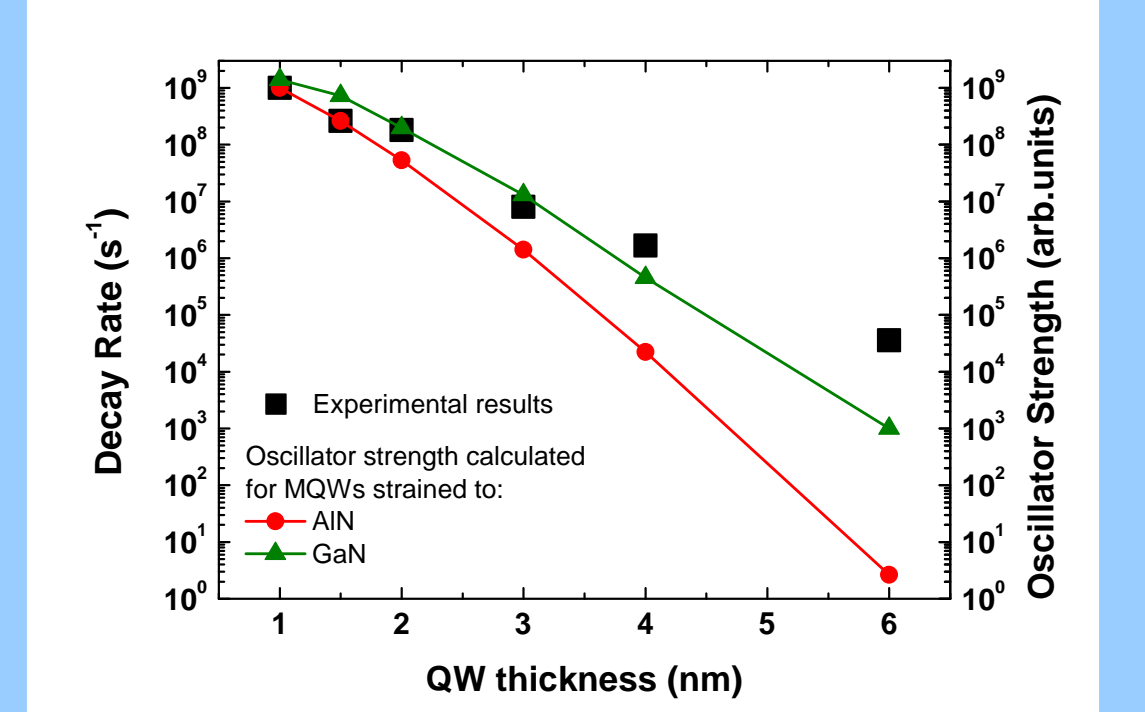


Recombination energy



- Various widths GaN/AIN MQWs
- Ab initio band-to-band transitions
- Experiment (◆)

Recombination rates



- Various widths GaN/AIN MQWs
- Ab initio band-to-band transitions
- Experiment (■)

Multiquantum well devices – LDs & LEDs

Drift-diffusion equations – discontinuous Galerkin method

$$-\nabla \cdot (\epsilon \nabla \psi) = \rho - \nabla \cdot P_0$$

$$-\nabla \cdot (\mu_n n \nabla F_n) = -qR$$

$$-\nabla \cdot (\mu_p p \nabla F_p) = qR$$

$$\rho = p - n + N_d^+ - N_a^-$$

$$n(x) = N_c \cdot \exp\left(\frac{F_n(x) - E_c + q\psi(x)}{kT}\right)$$

$$p(x) = N_v \cdot \exp\left(\frac{E_v - F_p(x) - q\psi(x)}{kT}\right)$$

$$N_d^+(x) = N_d \left[1 + g_d \exp\left(\frac{F_n(x) - E_c + E_d + q\psi(x)}{kT}\right) \right]$$

$$N_a^-(x) = N_a \left[1 + g_a \exp\left(\frac{E_v + E_a - F_p(x) - q\psi(x)}{kT}\right) \right]$$

$$R_{ABC}(x, N) = AN + BN^2 + CN^3$$

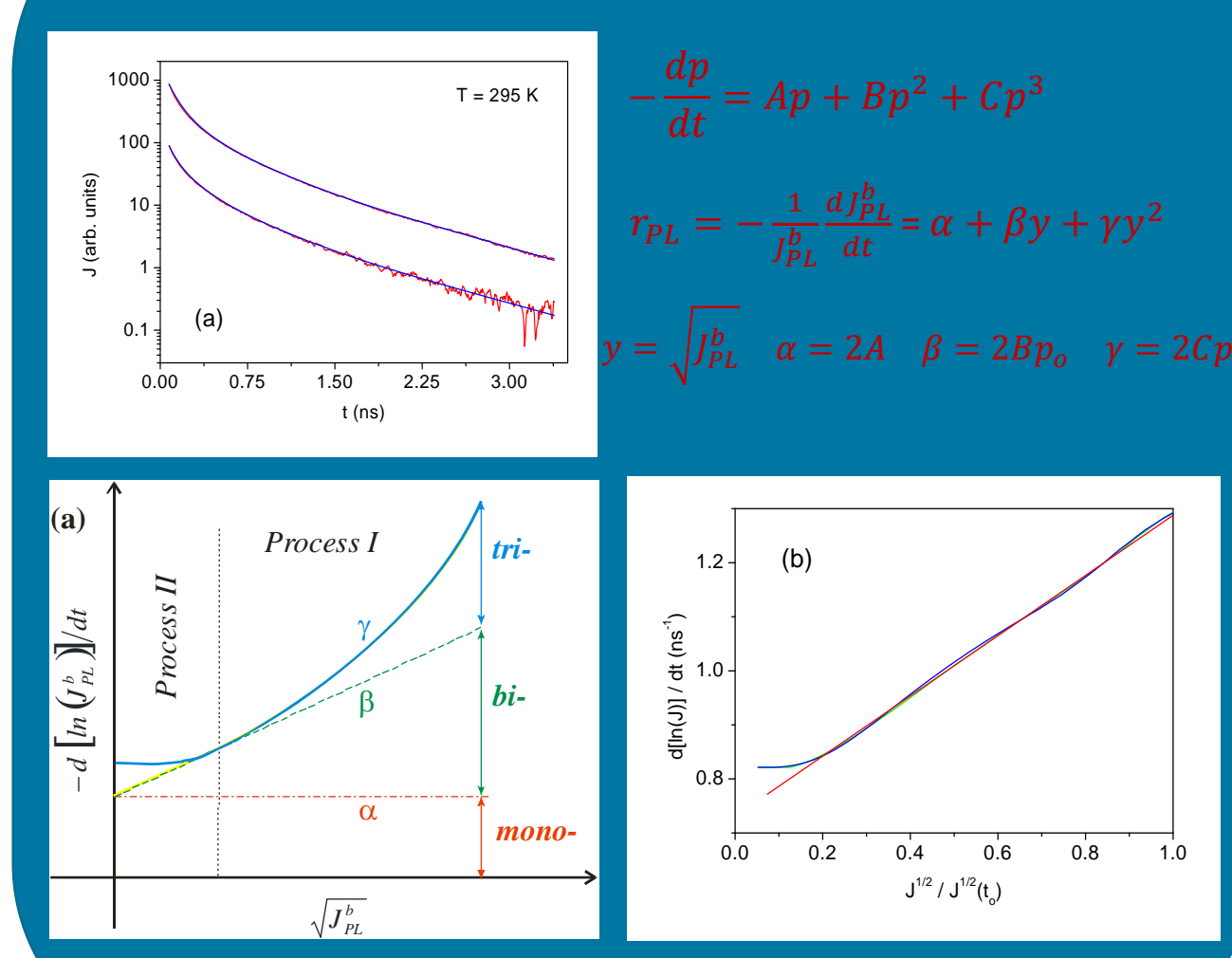
Poisson & continuity eqs

Mobile charge density

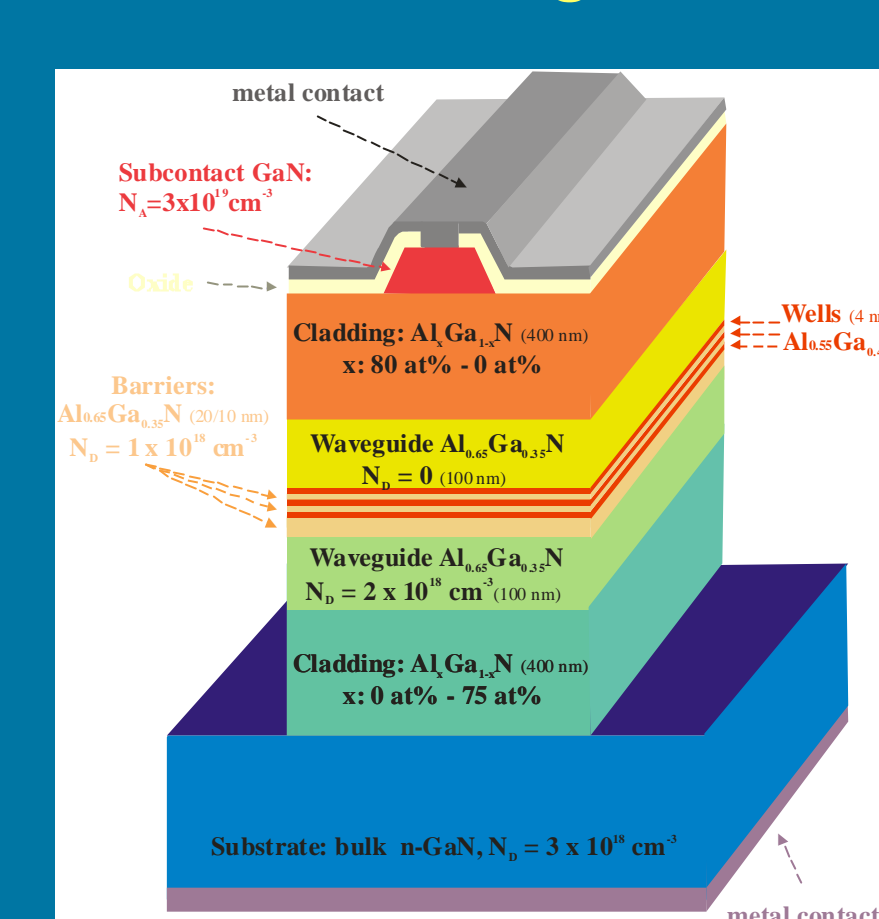
Defects

Recombination

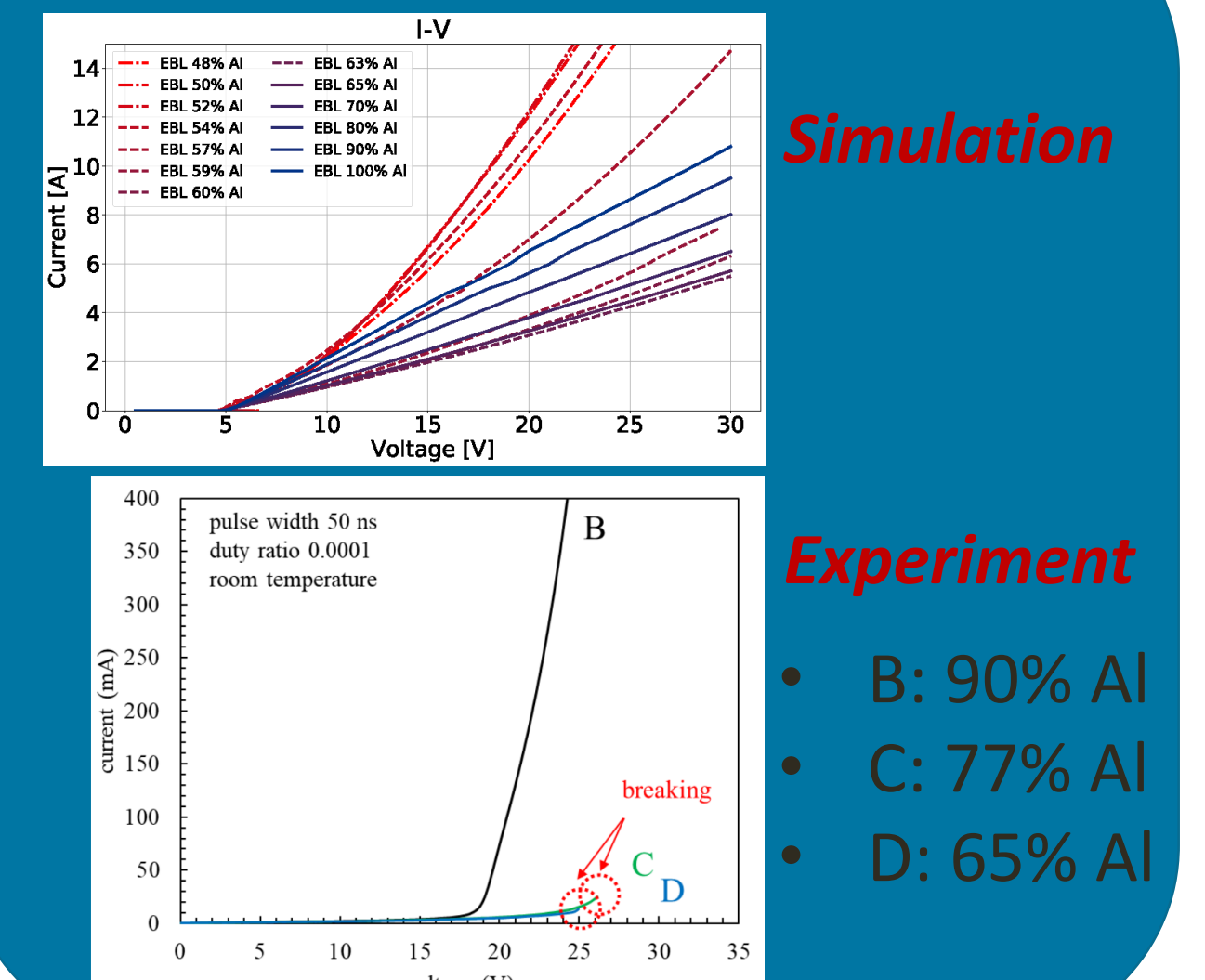
TRPL - decay constants (ABC)



LD design

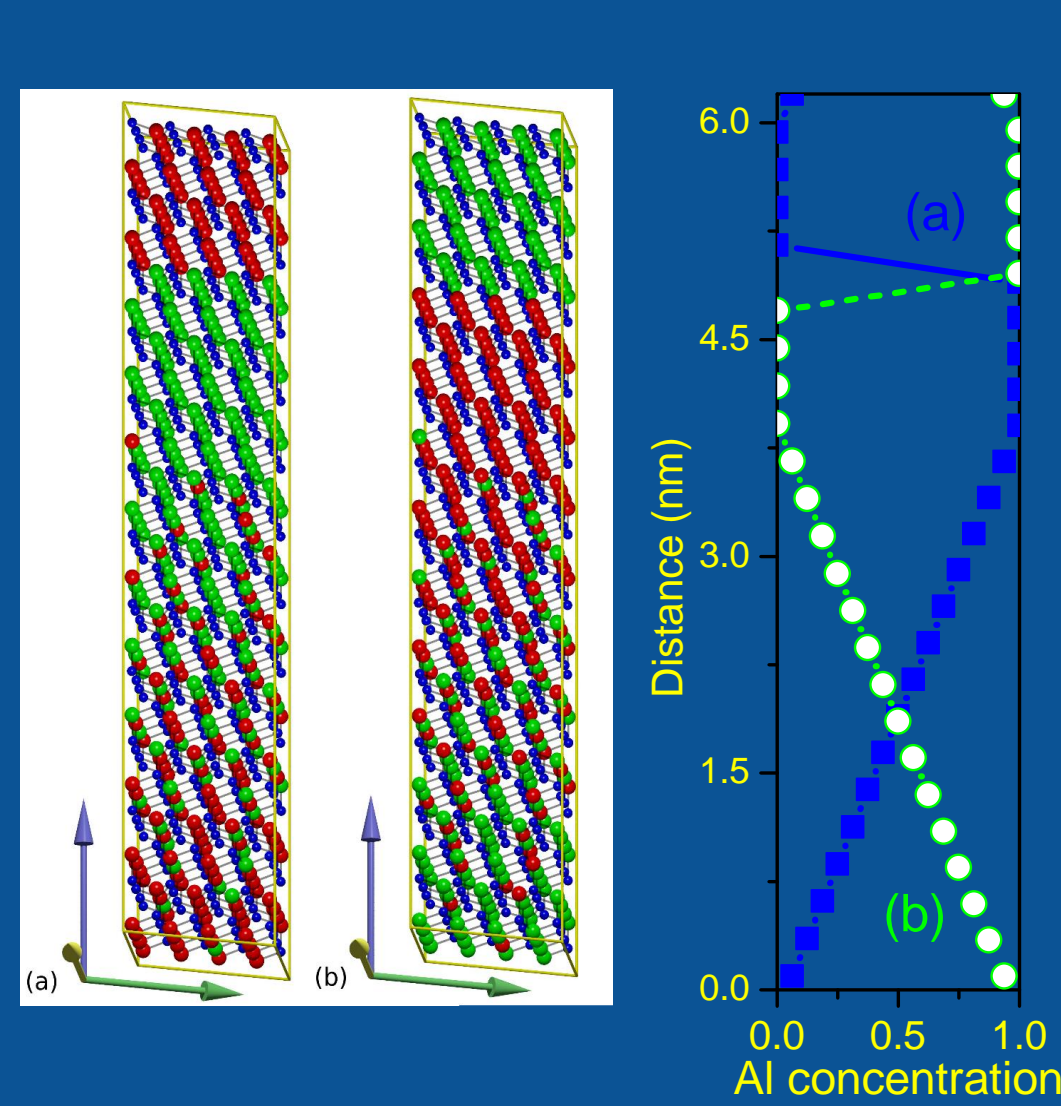


EBL – Al content

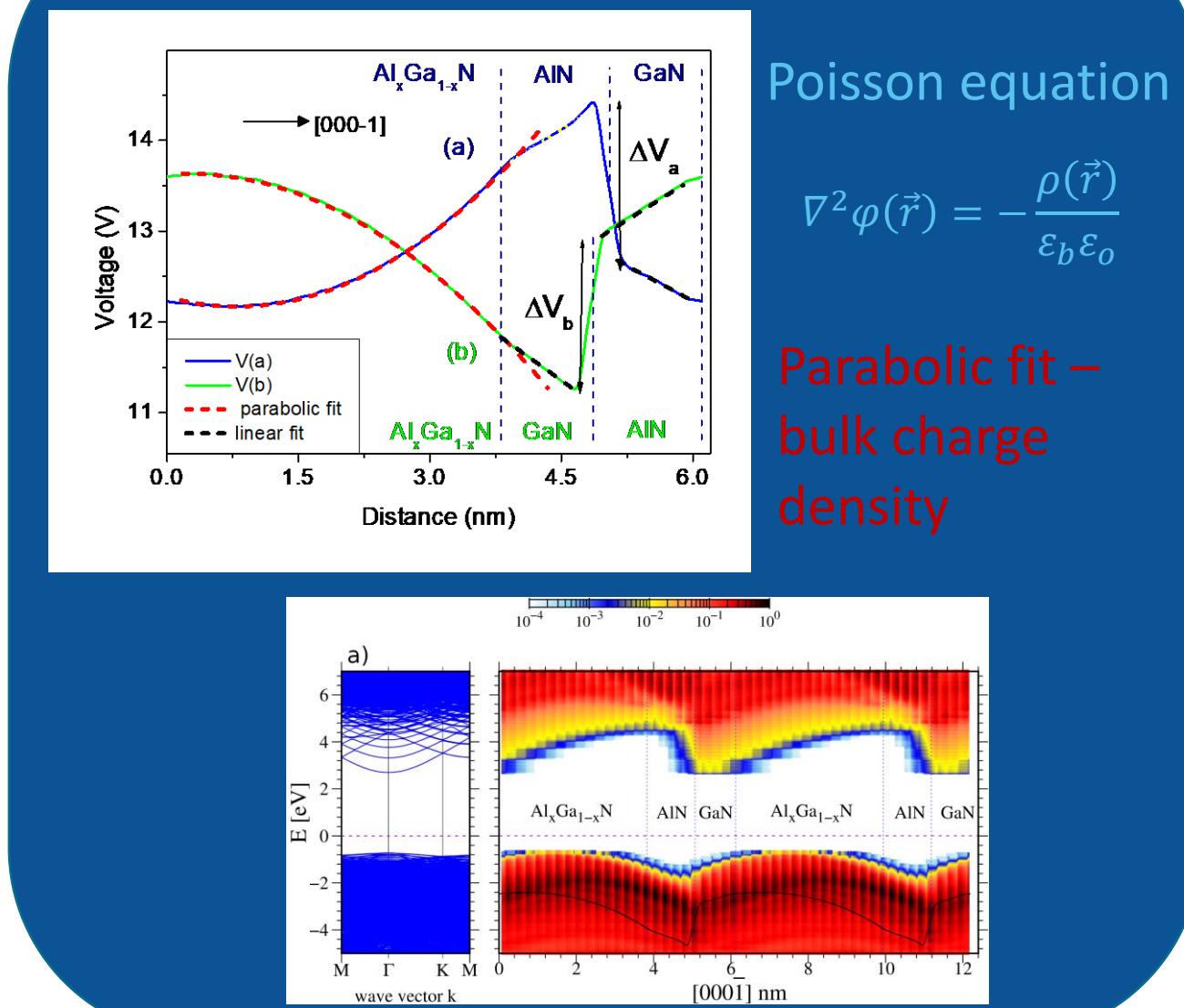


Polarization doping – route to UV devices

Atomic model of graded system



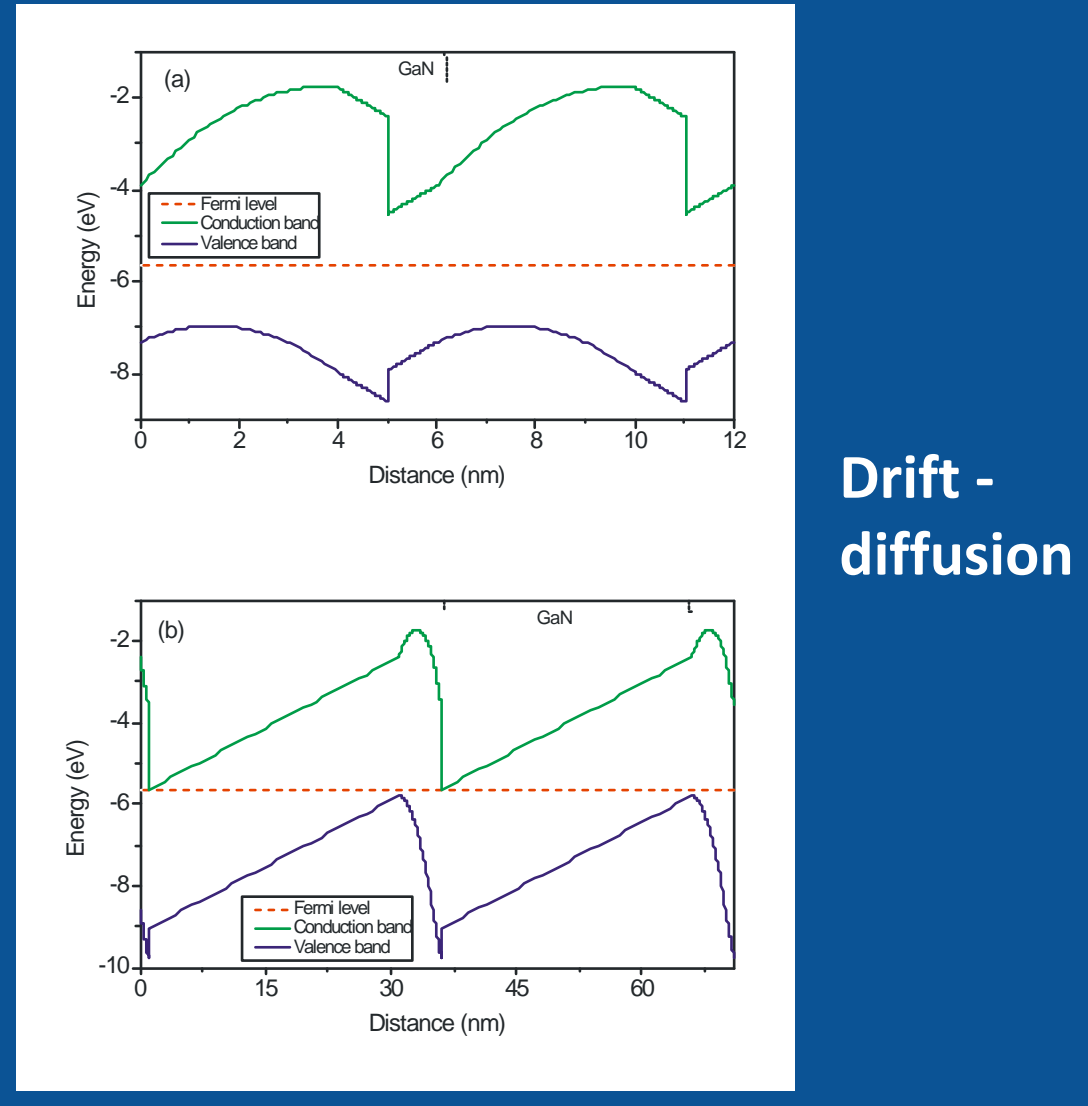
The potential and band profiles



$$\nabla^2 \varphi(\vec{r}) = -\frac{\rho(\vec{r})}{\epsilon_b \epsilon_0}$$

Parabolic fit – bulk charge density

Emergence of mobile charge



Drift - diffusion

Summary

- Model of determination of spontaneous polarization
- Averaging procedures for *ab initio*
- Nitride MWQs optical properties
- TRPL based procedure for determination of recombination parameters
- Drift-diffusion equation solution by discontinuous Galerkin method
- Existence of polarization doping charge
- Emergence of mobile charge in polarization doping systems

Use this QR code to see the poster on-line

