Polarization Effects in Heterojunction Band Offset Measurements of the ZnO-GaN Interface

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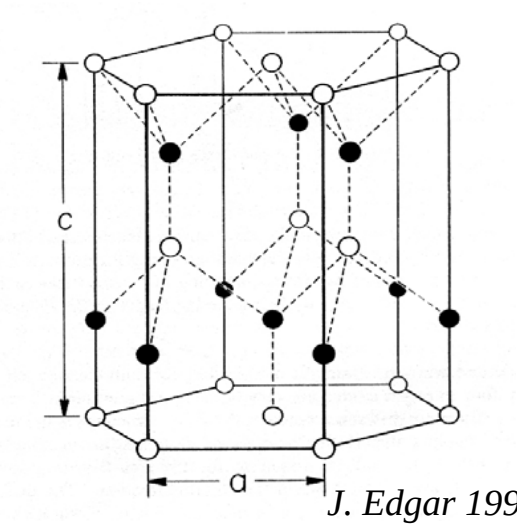
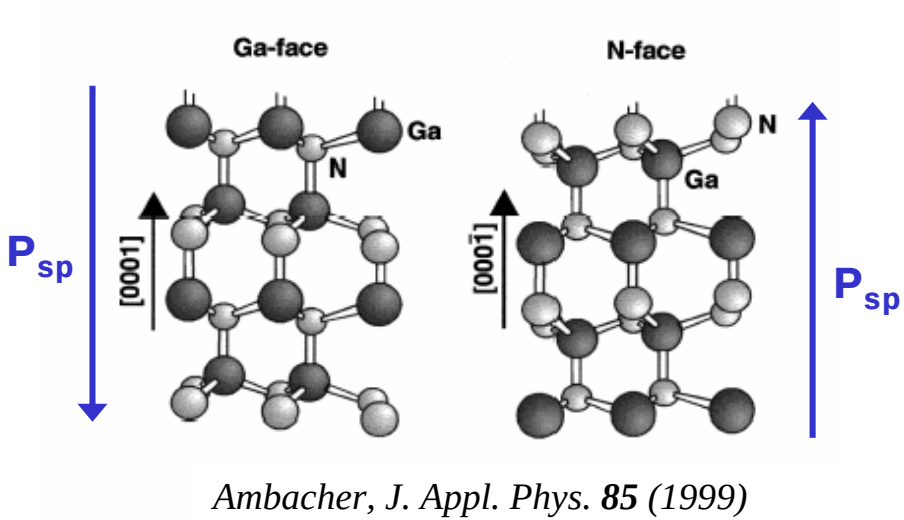
Polarization Band Bending Effects



J. Edgar 1994

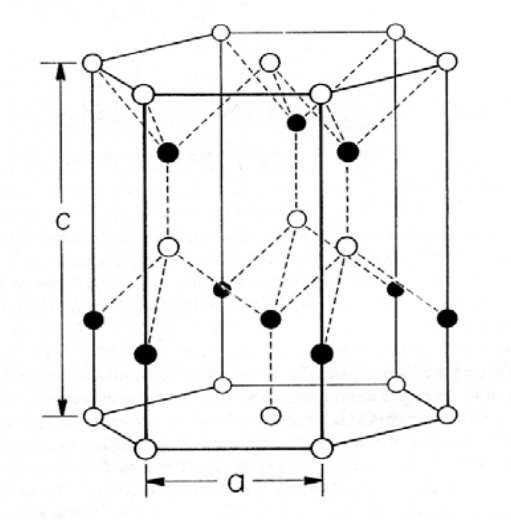


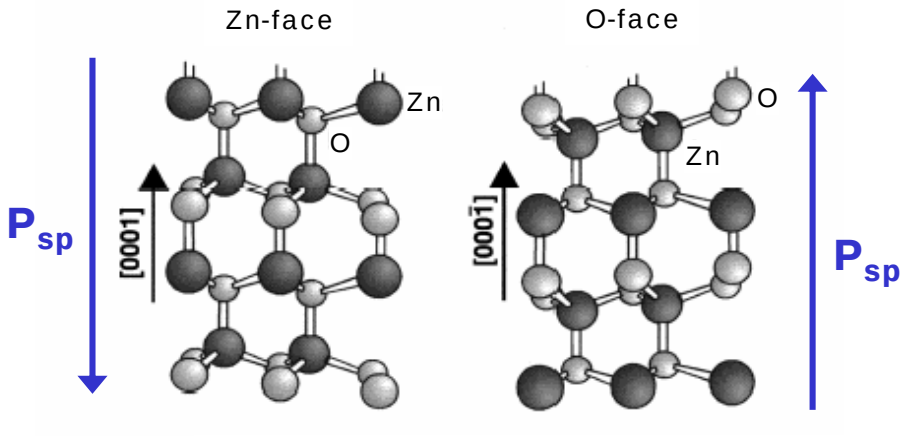
Ambacher, J. Appl. Phys. ***85*** *(1999)*

- GaN is a polar crystal
- P_{SP} = -0.034 C/m^2, Polarization bound charge is 2.12x10^{13} cm^{-2} *
- Spontaneous polarization leads to
  - negative bound charge at the (0001) Ga face
  - positive bound charge at (000-1) N face

* *Zoroddu et al., Phys. Rev. B* ***64*** *045208*

Polarization Band Bending Effects



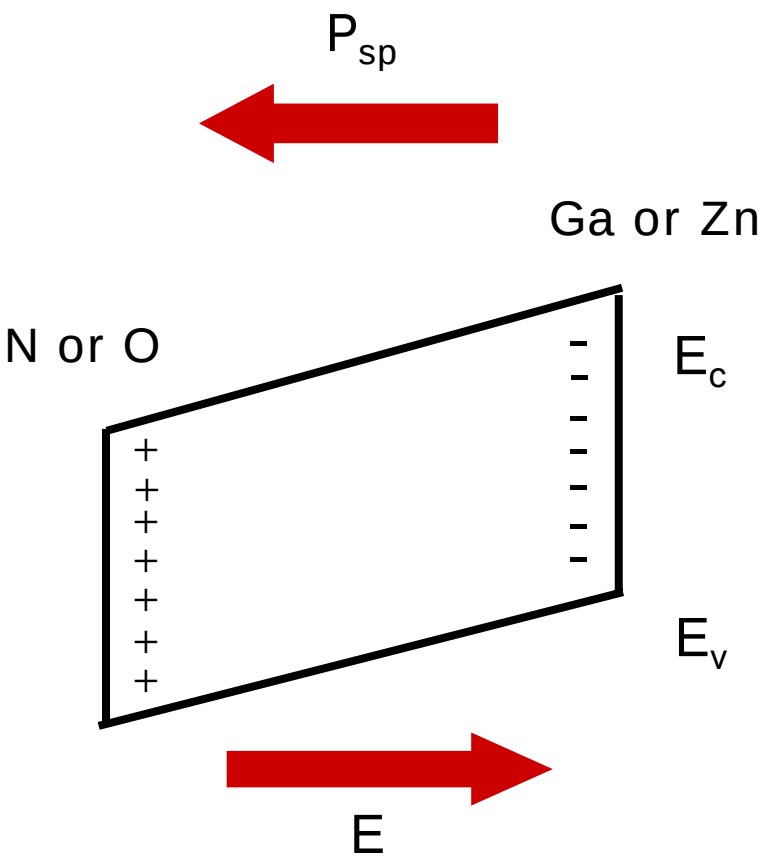


Xu, Appl. Phys. Lett. ***84*** *(2004)*

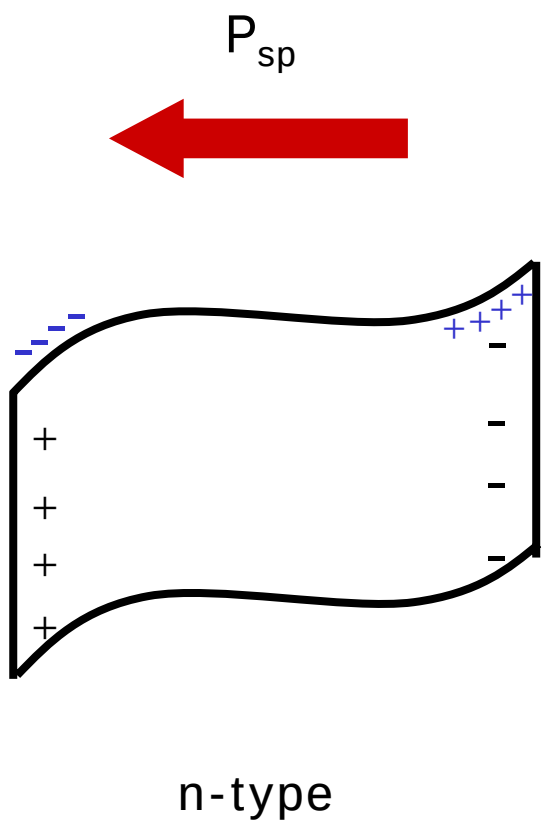
- ZnO is also a polar crystal
- P_{SP} = -0.057 C/m^2, Polarization bound charge is 3.56x10^{13} cm^{-2} *
- Spontaneous polarization leads to
  - negative bound charge at the (0001) Zn face
  - positive bound charge at (000-1) O face

* *Bernardini et al., Phys. Rev. B* ***56*** *R10024*

Role of Free Carriers

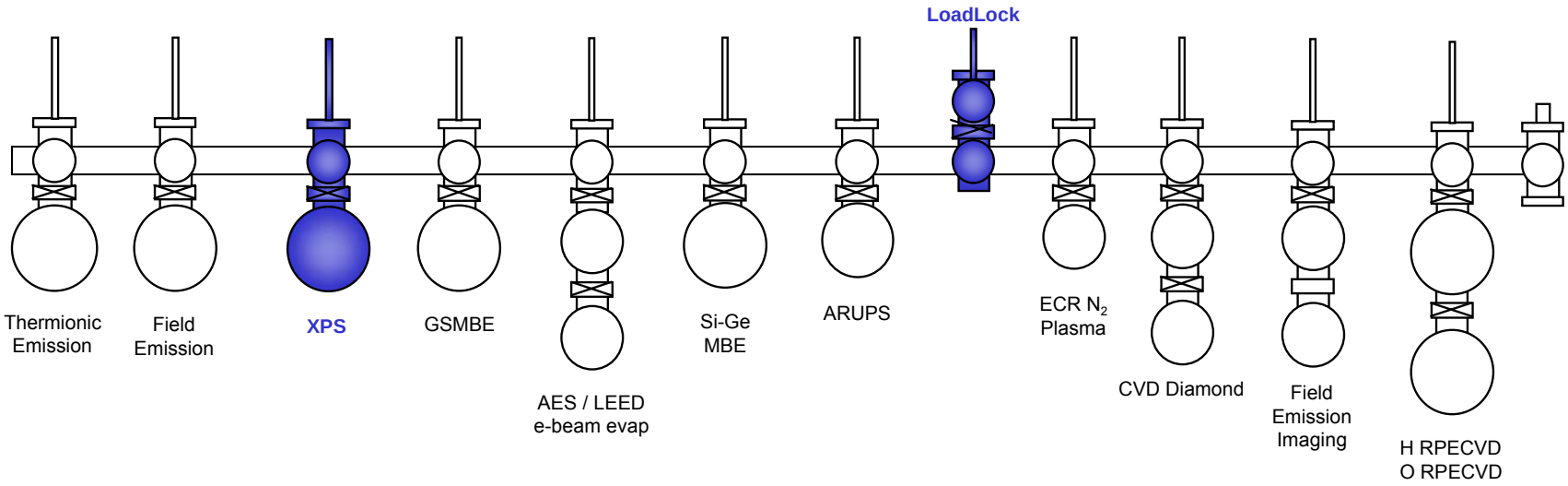


Internal electric field due to spontaneous polarization



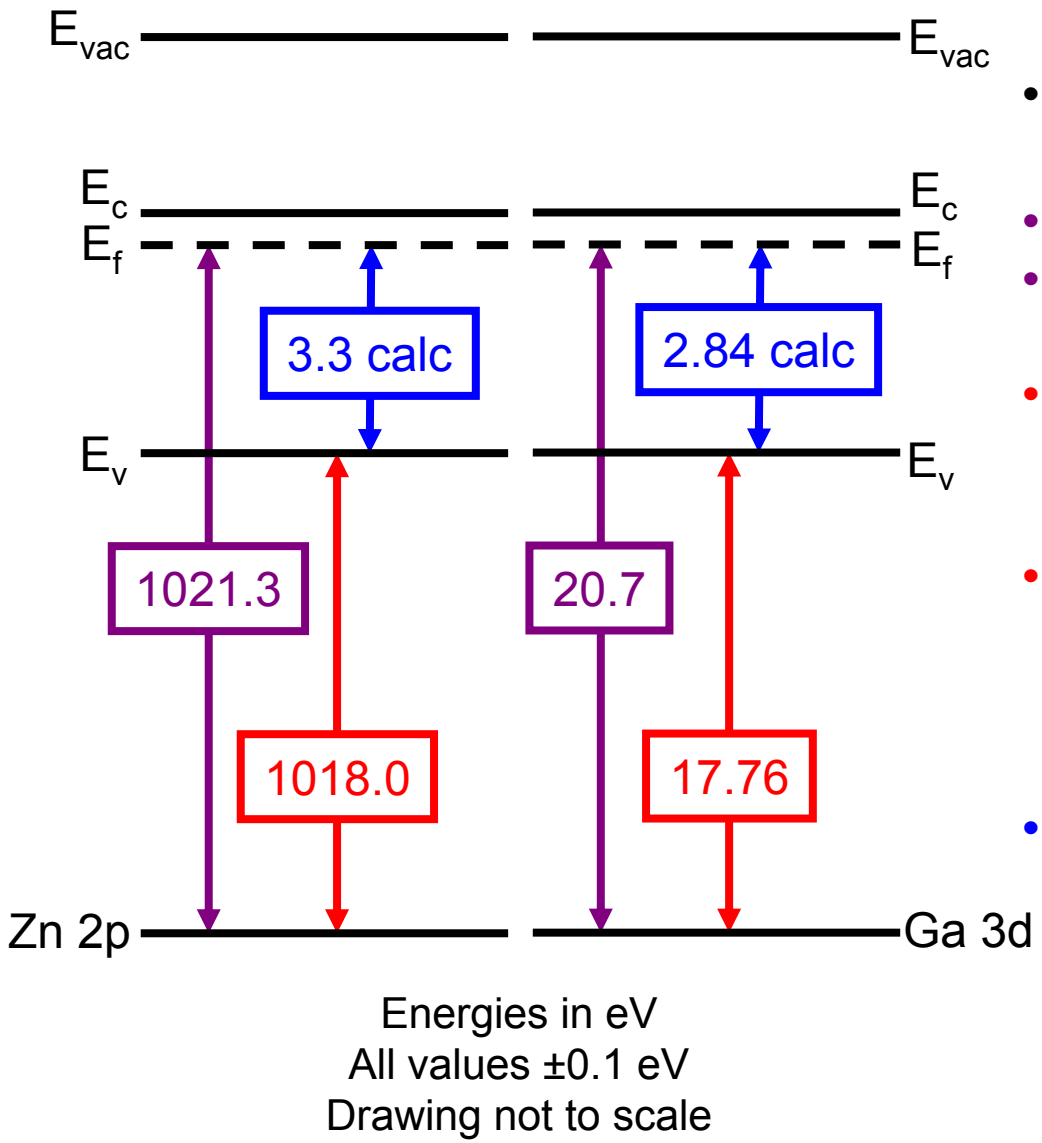
Free carriers screen the polarization bound charge

Experimental Technique



- UHV measurements
- Core level position related to VBM position
- XPS Core level spectra
  - Ga 3d gives GaN VBM
  - Zn 2p gives ZnO VBM

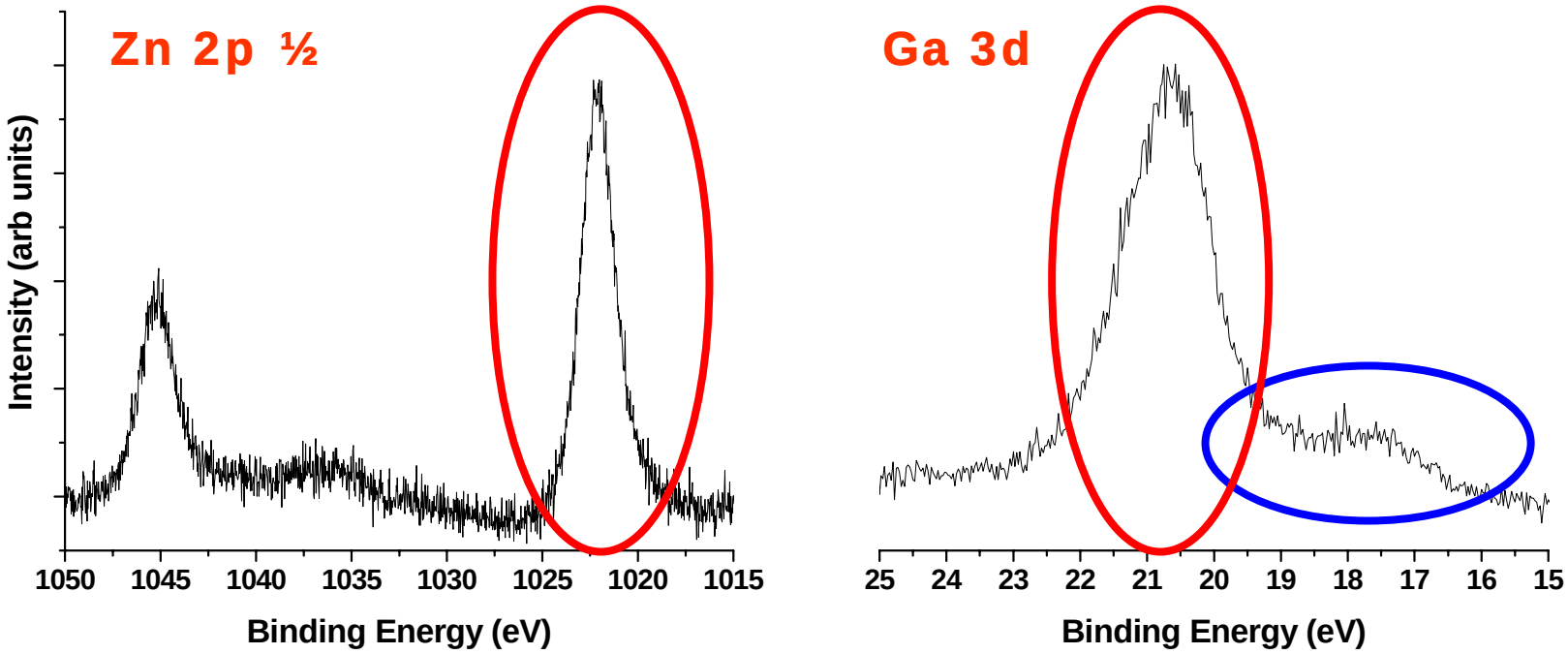
Valence Band Maximum Determination



Energies in eV
All values ±0.1 eV
Drawing not to scale

- Schematic of bands
- [E_f → Ga 3d] measured by XPS
- [E_f → Zn2p ½] measured by XPS
- [E_v → Ga3d] constant of GaN
  - *Waldrop and Grant APL 68 (1996)*
- [E_v → Zn2p ½] constant of ZnO
  - *B. J. Coppa, et al. JAP, 95, (2004)*
- E_f → E_v calculated

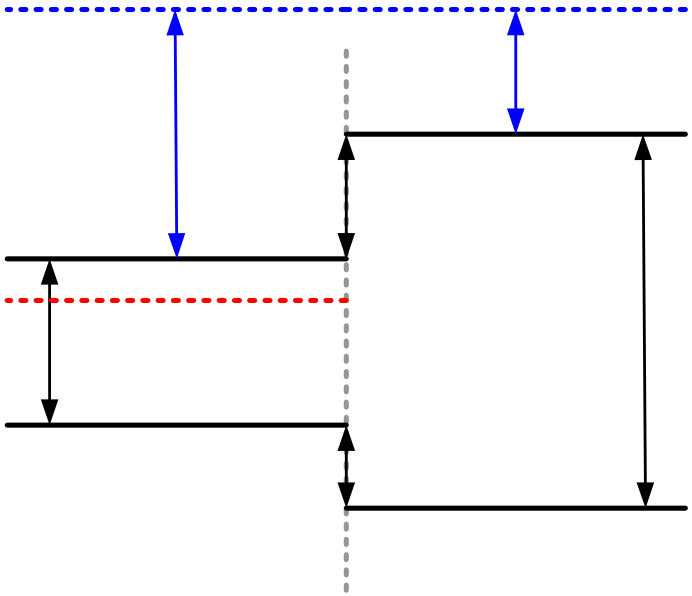
XPS Core Level Spectra



- Core levels give only relative valence band positions
  - charging effects both Ga and Zn core levels equally
  - no absolute measure of E_F or band bending

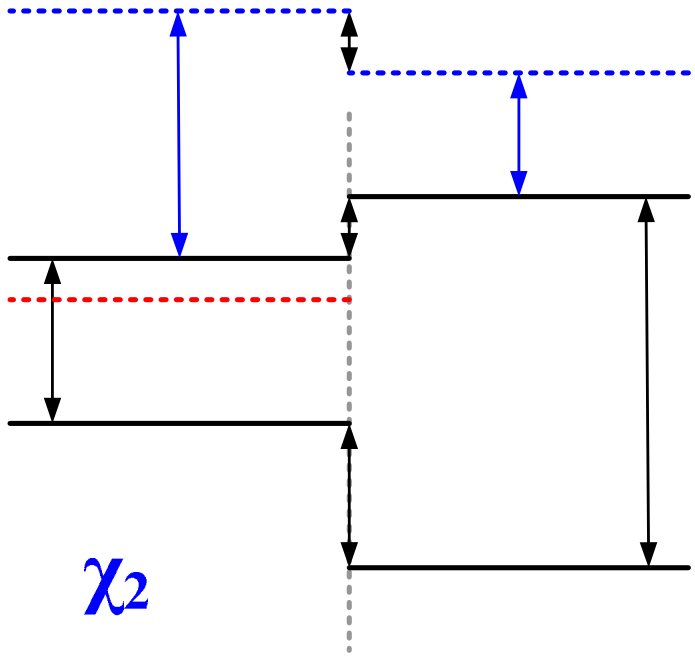
- Possible gallium oxide at the interface

Interface Models



- Electron Affinity Model*
  - align electron affinities

$$\phi_{CBO} = (\chi_1 - \chi_2)$$

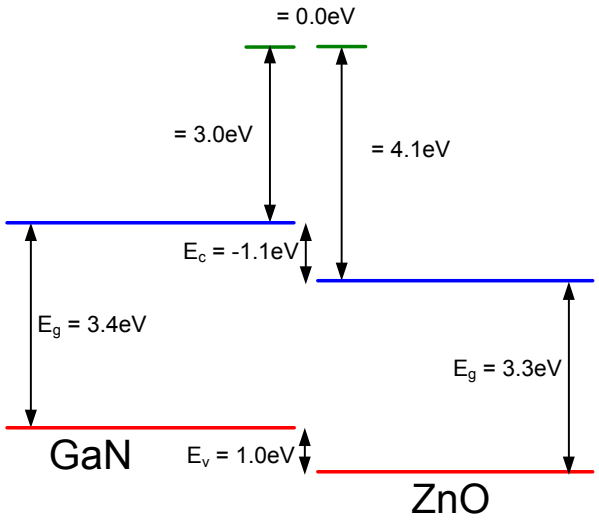


- Charge Neutrality Model†
- Align charge neutrality levels
- Charge transfer between interface states
  - deviation from electron affinity model
  - interface dipole (Δ)

$$\phi_{CBO} = (\chi_1 - \chi_2) \pm \Delta$$

* Anderson *et al.*
† Tersoff, Mönch, Robertson

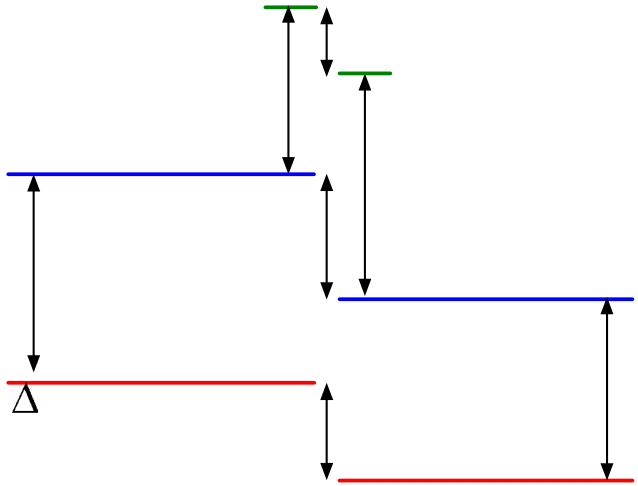
Ga-face GaN – ZnO



χ

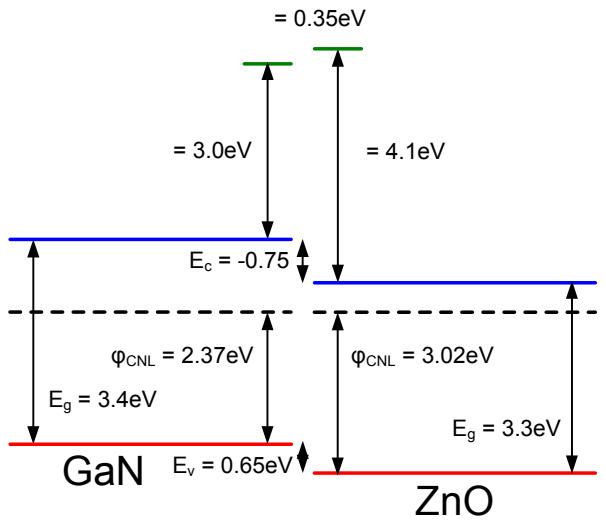
- EAM
  - no dipole

Δ



χ

- Measured
  - dipole = -0.85eV



χ = 3.0e

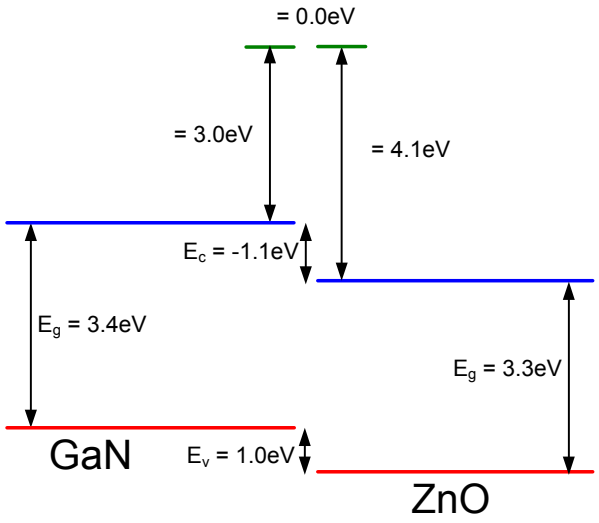
- CNL*
  - dipole = +0.35eV

ΔE_c = -1.

E_g = 3.4eV

* W. Mönch, Universität Duisburg-Essen

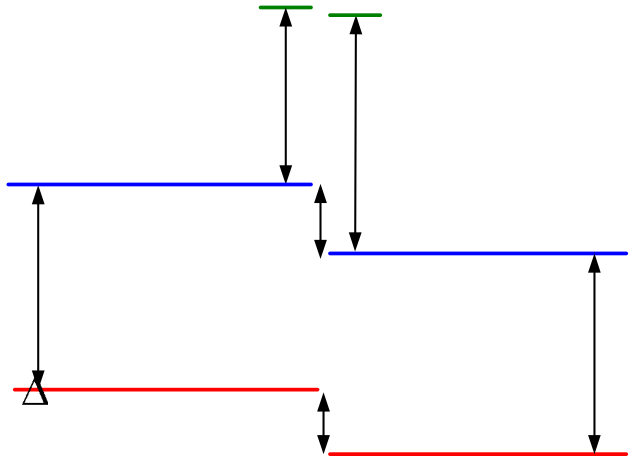
N-face GaN – ZnO



χ

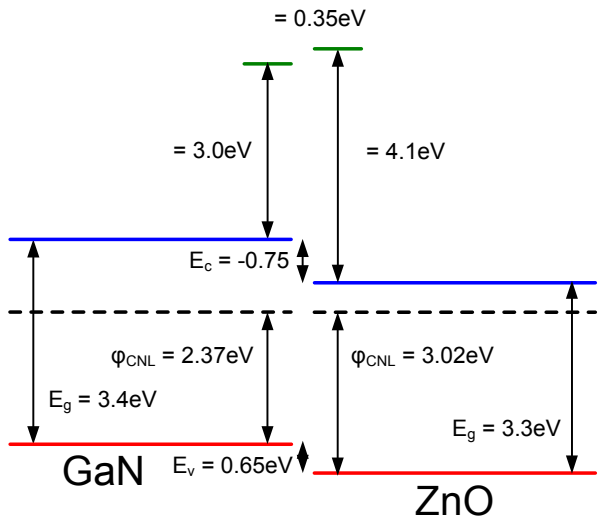
- EAM
  - no dipole

Δ



χ

- Measured
  - dipole = -0.05eV



χ = 3.0eV

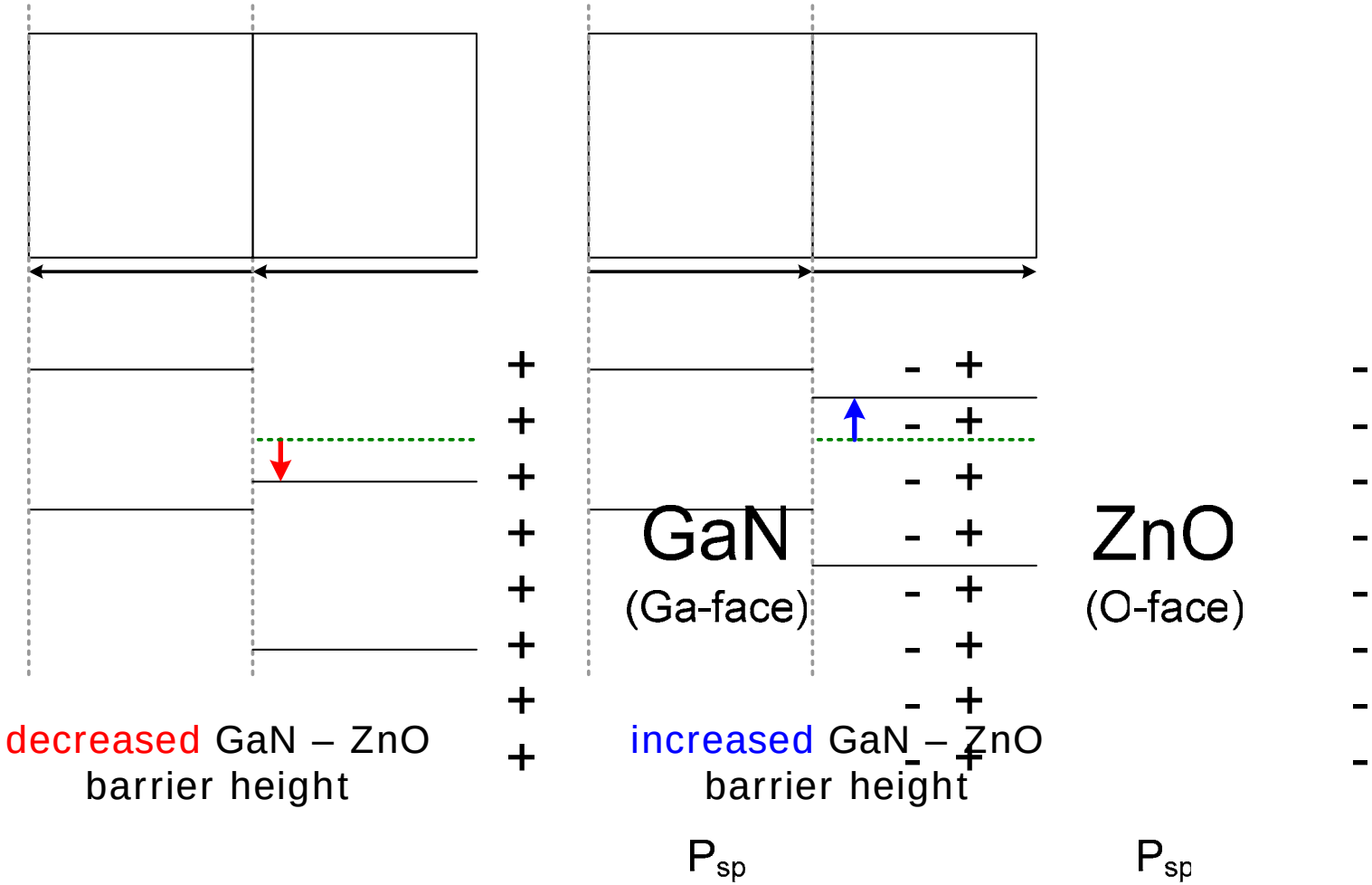
- CNL*
  - dipole = +0.35eV

ΔE_c = -1.15

E_g = 3.4eV

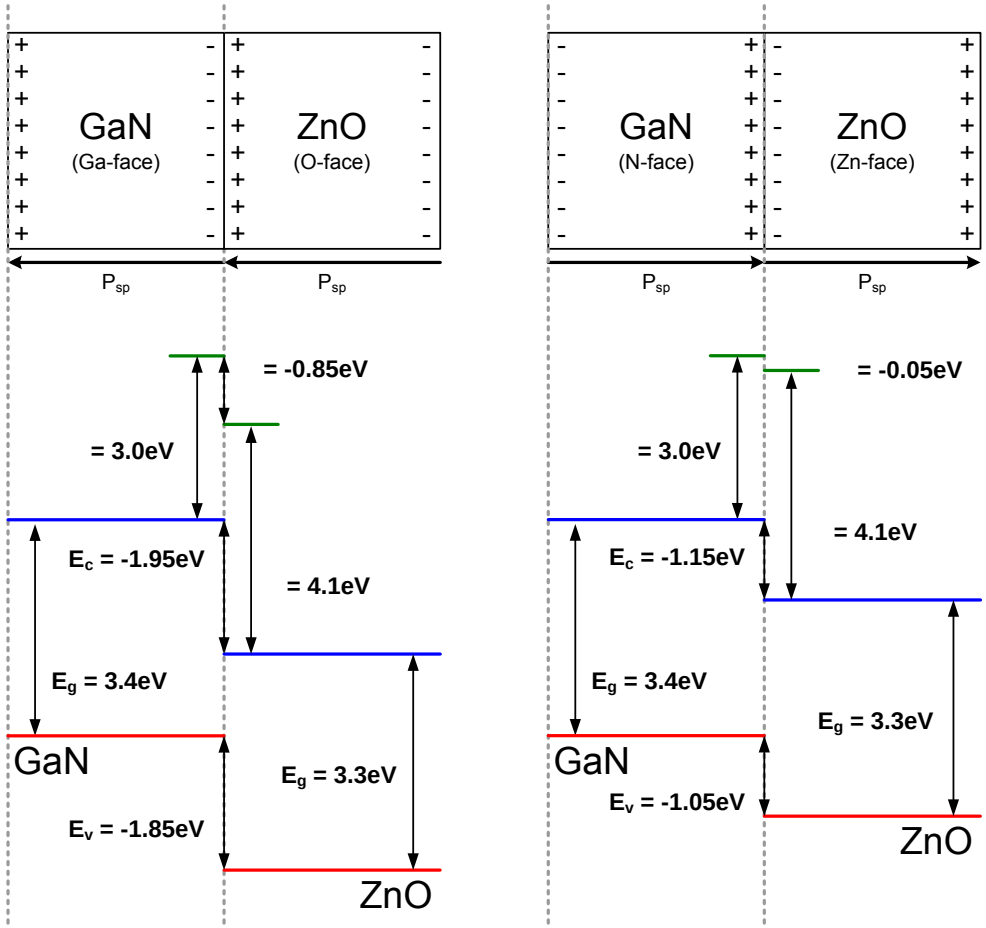
* W. Mönch, Universität Duisburg-Essin

Suggested Interface Structure



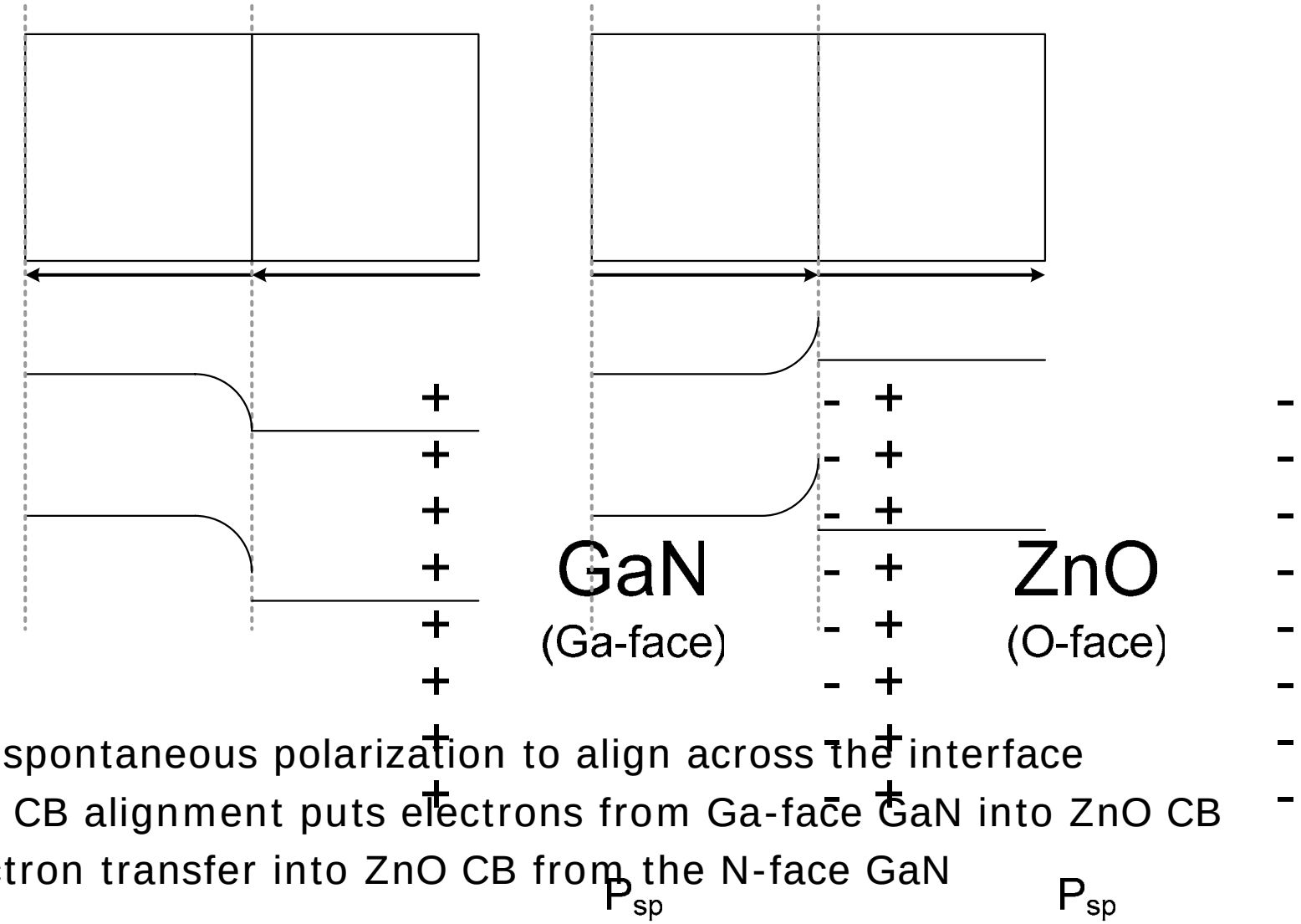
- GaN and ZnO are both polar materials
- Expect spontaneous polarization to align across the interface
- Direction of interface dipoles can increase or decrease barrier height

Suggested Interface Structure



- Direction of band offset difference is consistent with a polarization induced interface dipole.

Interface Structure Including Free Carriers



- Expect spontaneous polarization to align across the interface
- Type II CB alignment puts electrons from Ga-face GaN into ZnO CB
- No electron transfer into ZnO CB from the N-face GaN

Conclusions

- GaN polarity plays a significant role in band alignment and interface electronic structure
  - Ga-face - interface dipole of -0.85 eV
  - N-face - interface dipole of -0.05 eV
- N-face results consistent with electron affinity model
- Ga-face results do not fit with either EA or CNL models
  - models do not include polarity contribution
  - gallium oxide may exist at the interface
- Band offset difference between Ga-face and N-face is consistent with polarization induced interface dipole.

Questions

- Can we verify the polarity of the GaN-ZnO interface?
- Do polarity induced bound charges contribute to the energetics of the interface bonding? And the band offsets?
- Can we quantify the effects of gallium oxide at the interface?
- What is the net polarization bound charge at the interface? And what is the role of defects?