

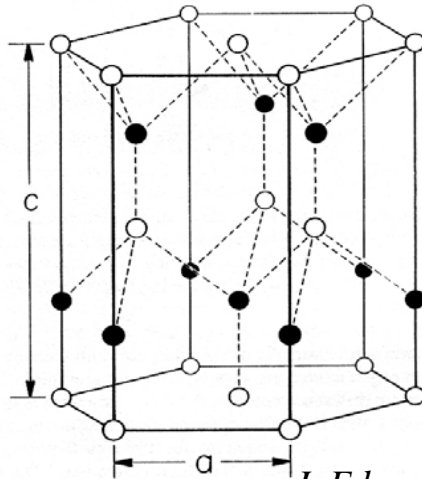
Polarization Effects in Heterojunction Band Offset Measurements of the ZnO-GaN Interface

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Sang-Jun Cho³, H. Morkoç³

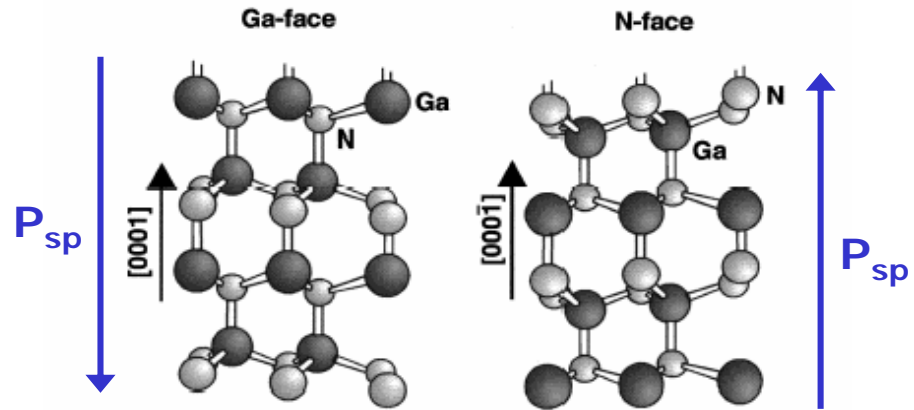
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Richmond, Virginia 23284

Polarization Band Bending Effects



J. Edgar 1994

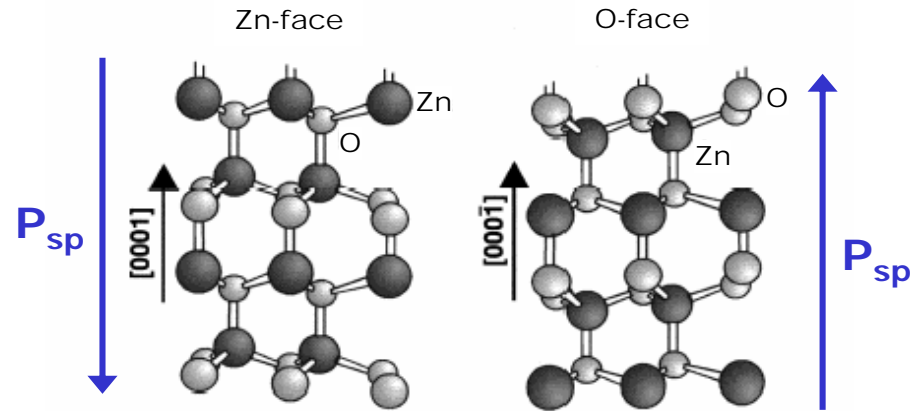
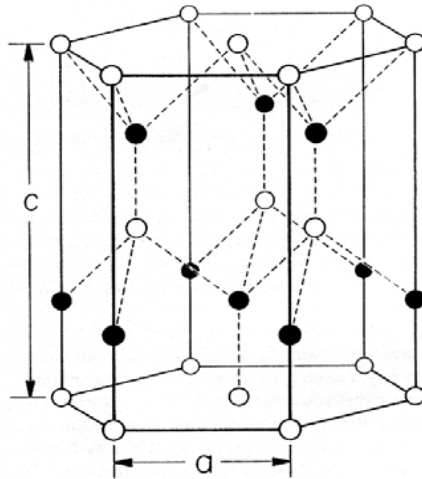


Ambacher, J. Appl. Phys. 85 (1999)

- GaN is a polar crystal
- $P_{sp} = -0.034 \text{ C/m}^2$, Polarization bound charge is $2.12 \times 10^{13} \text{ cm}^{-2}$ *
- 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

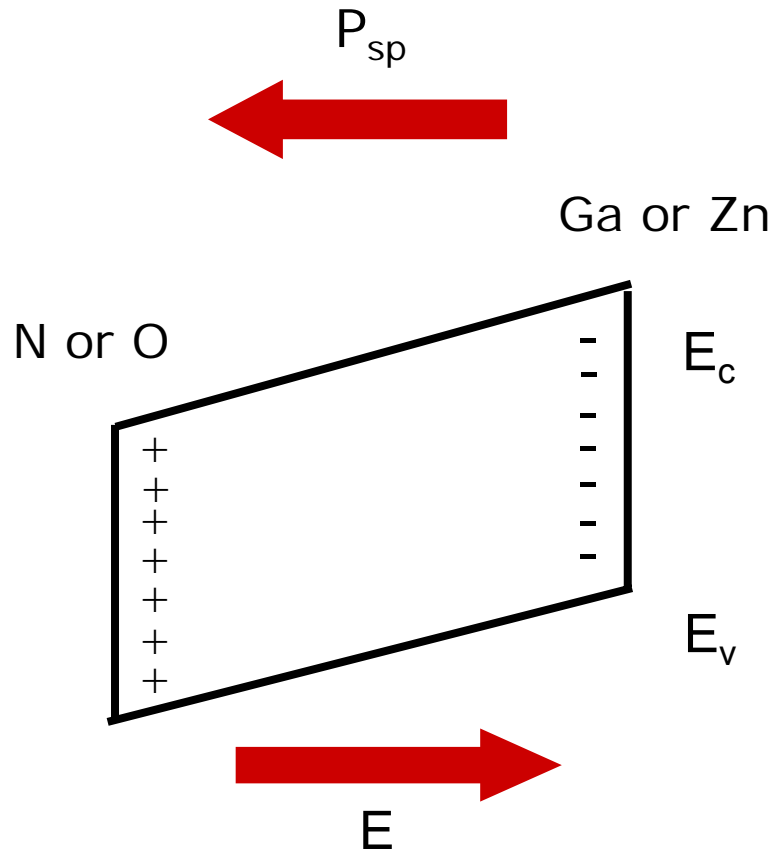


Xu, Appl. Phys. Lett. 84 (2004)

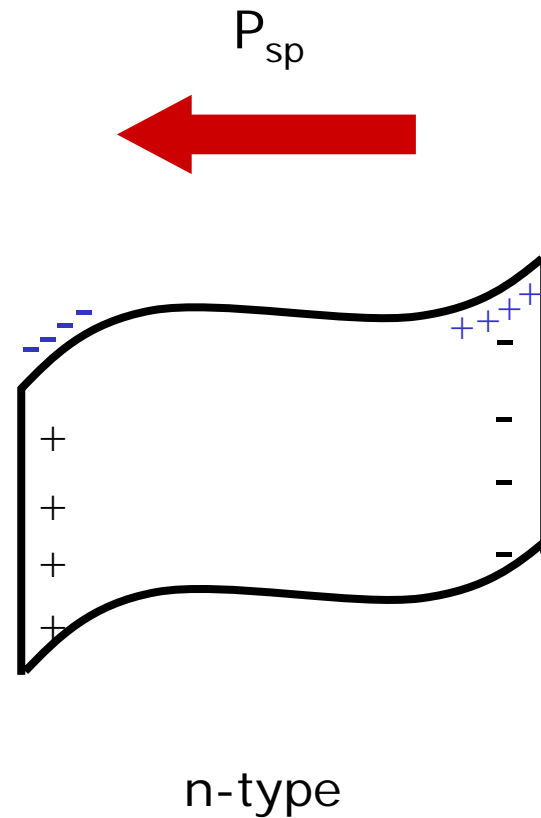
- ZnO is also a polar crystal
- $P_{sp} = -0.057 \text{ C/m}^2$, Polarization bound charge is $3.56 \times 10^{13} \text{ cm}^{-2}$ *
- Spontaneous polarization leads to
 - negative bound charge at the (0001) Zn face
 - positive bound charge at (000-1) O face

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

Role of Free Carriers

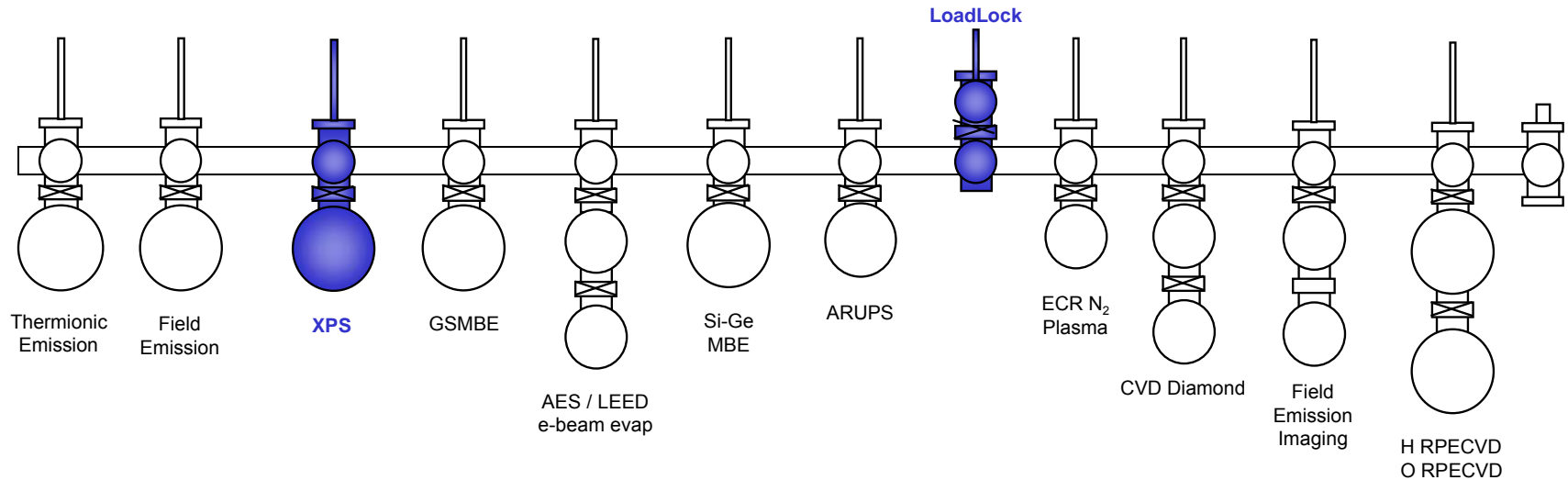


Internal electric field due to spontaneous polarization



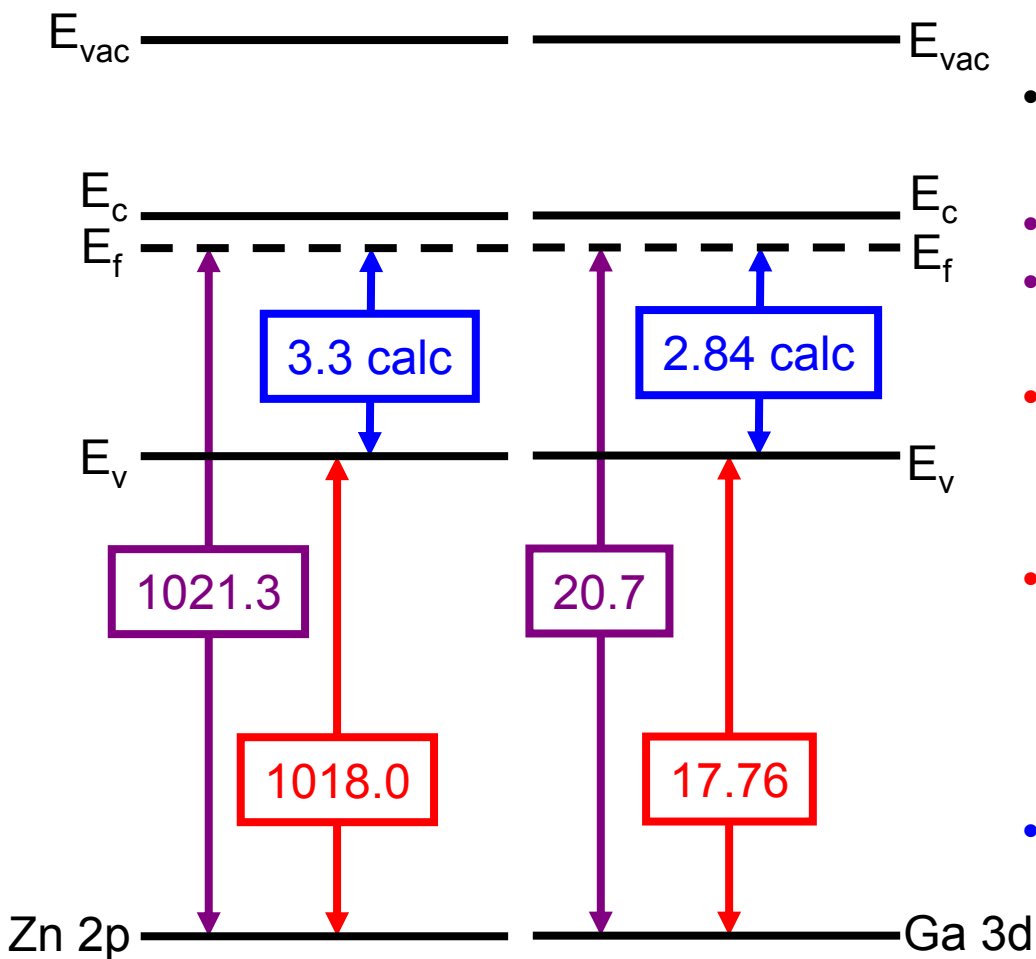
Free carriers screen the polarization bound charge

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

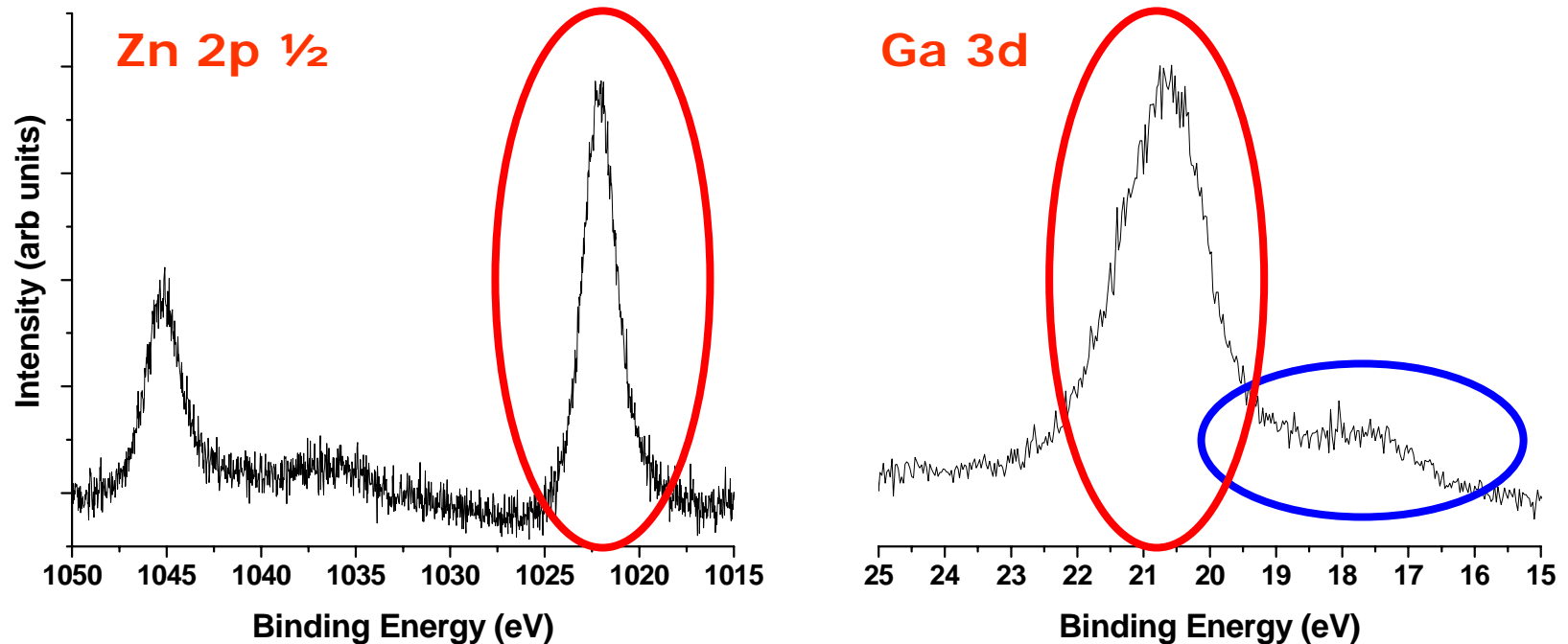
Valence Band Maximum Determination



- Schematic of bands
- $[E_f \rightarrow \text{Ga } 3d]$ measured by XPS
- $[E_f \rightarrow \text{Zn } 2p \frac{1}{2}]$ measured by XPS
- $[E_v \rightarrow \text{Ga } 3d]$ constant of GaN
 - Waldrop and Grant APL 68 (1996)
- $[E_v \rightarrow \text{Zn } 2p \frac{1}{2}]$ constant of ZnO
 - B. J. Coppa, et al. JAP, 95, (2004)
- $E_f \rightarrow E_v$ calculated

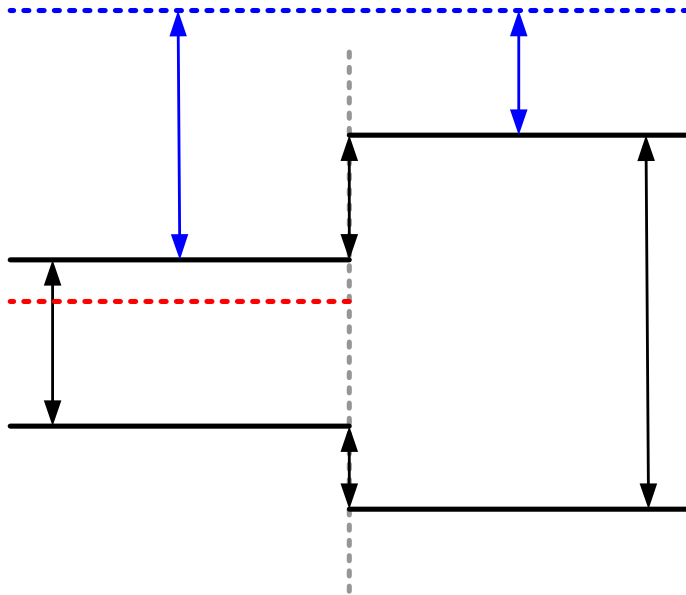
Energies in eV
All values ± 0.1 eV
Drawing not to scale

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

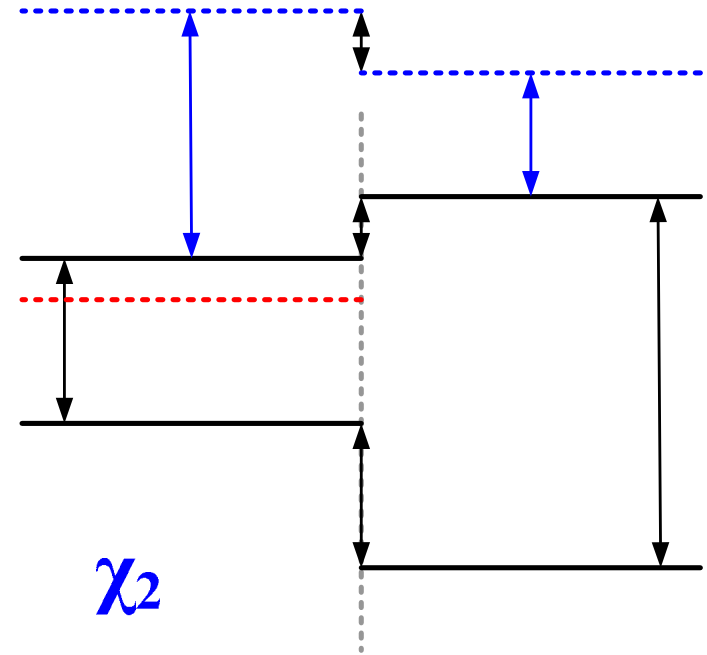


- Electron Affinity Model*
 - align electron affinities

E_c

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

E_{g1}



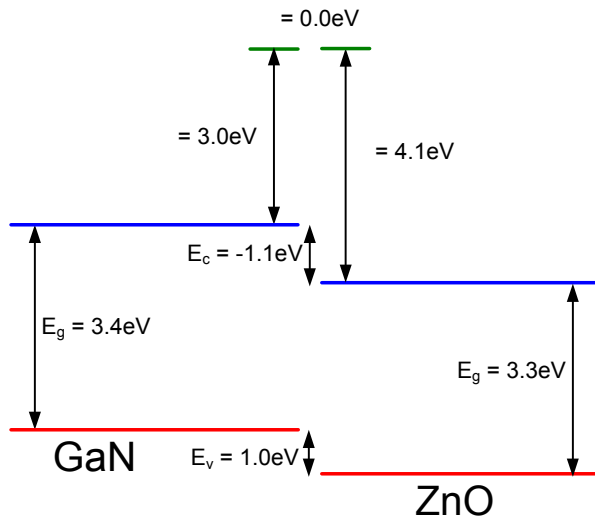
- Charge Neutrality Model†
- Align charge neutrality levels
- Charge transfer between interface states
 - deviation from electron affinity model
 - interface dipole (Δ)

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

* Anderson *et al.*

† Tersoff, Mönch, Robertson

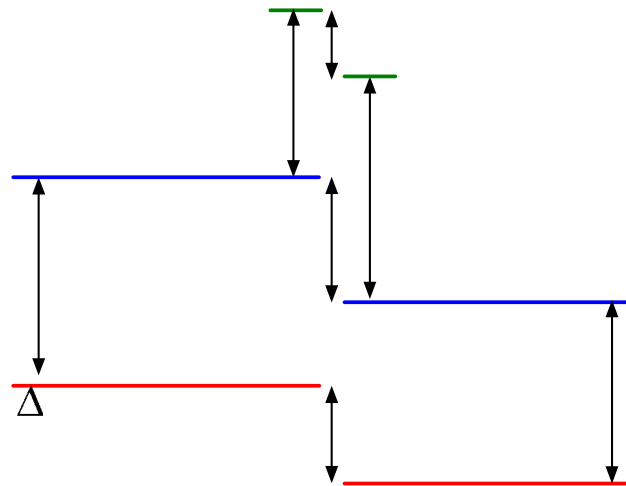
Ga-face GaN – ZnO



χ

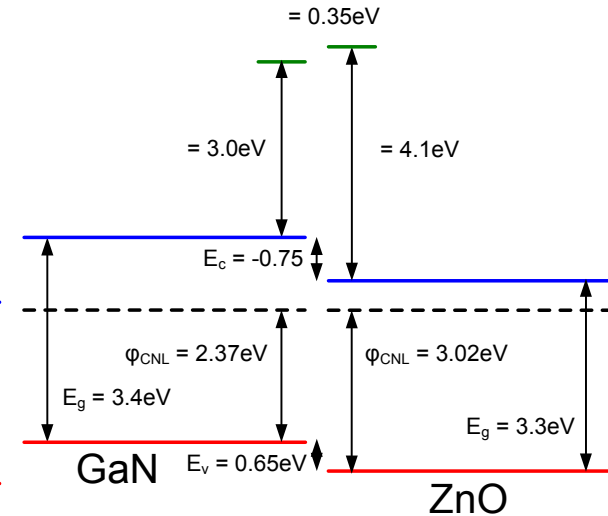
- EAM
 - no dipole

Δ



χ

- Measured
 - dipole = -0.85eV

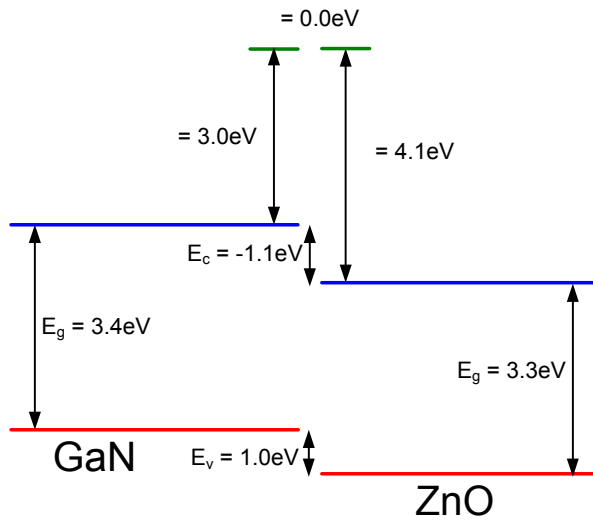


$\chi = 3.0\text{eV}$

- CNL*
 - dipole = $+0.35\text{eV}$
 - $\Delta E_c = -1.1\text{eV}$

$E_g = 3.4\text{eV}$

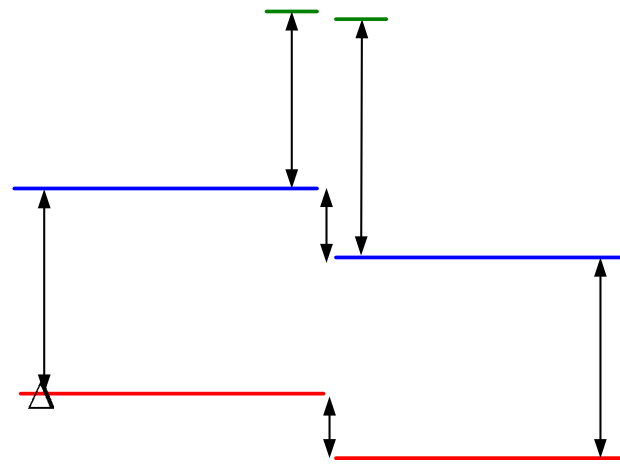
N-face GaN – ZnO



χ

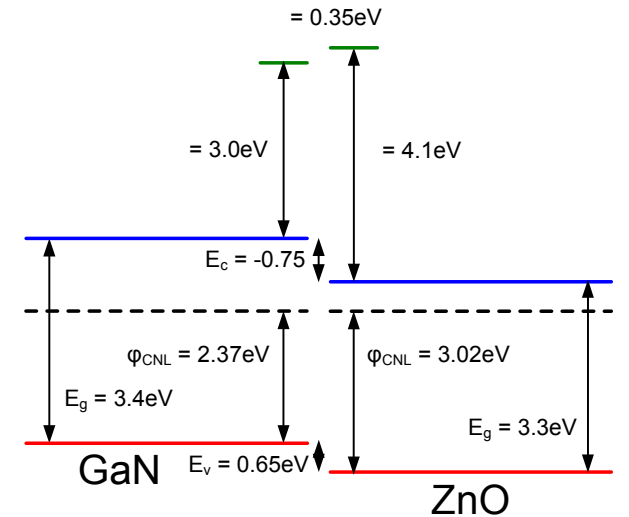
- EAM
 - no dipole

Δ



χ

- Measured
 - dipole = -0.05eV



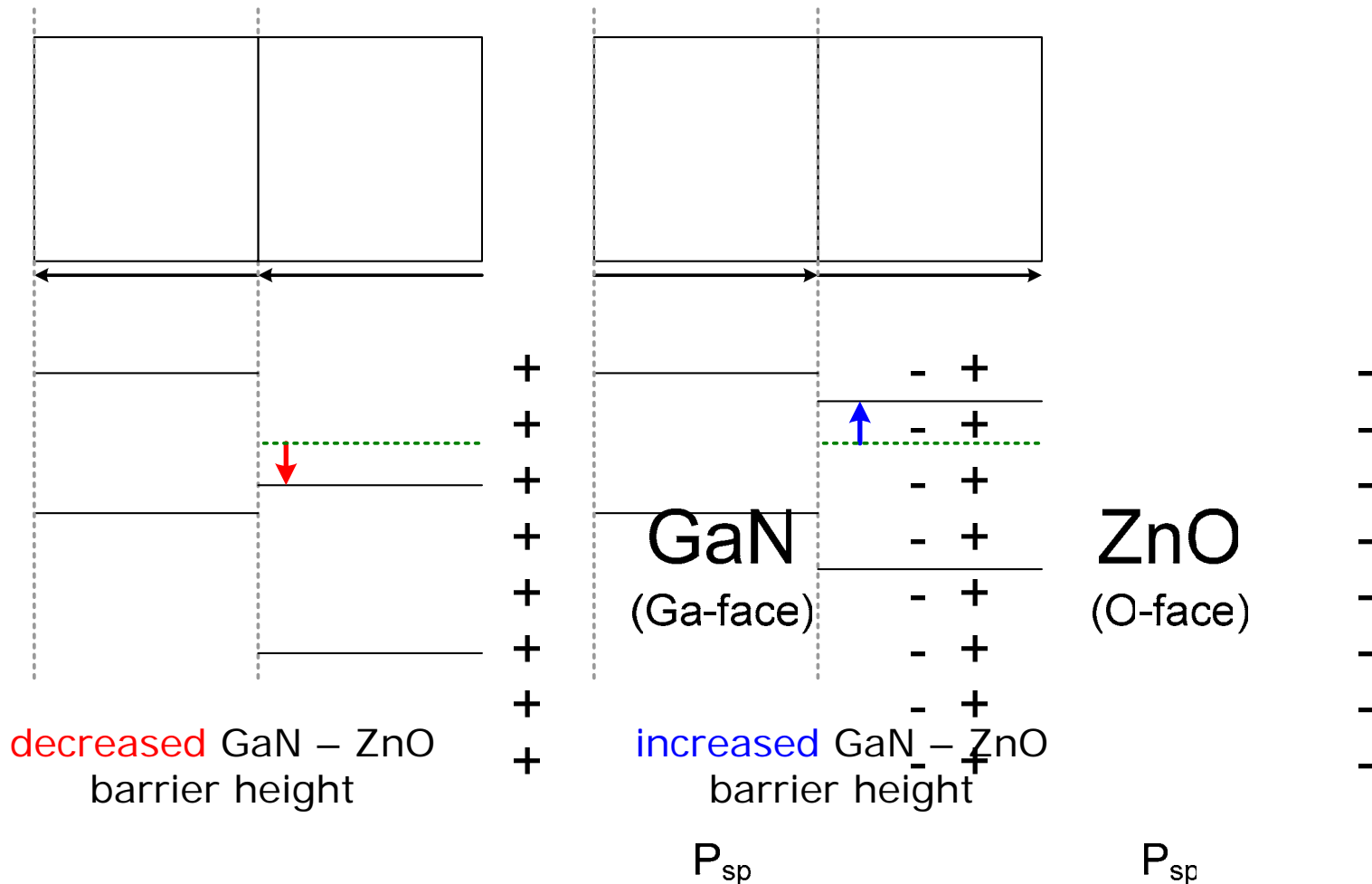
$\chi = 3.0\text{eV}$

- CNL*
 - dipole = $+0.35\text{eV}$

$E_g = 3.4\text{eV}$

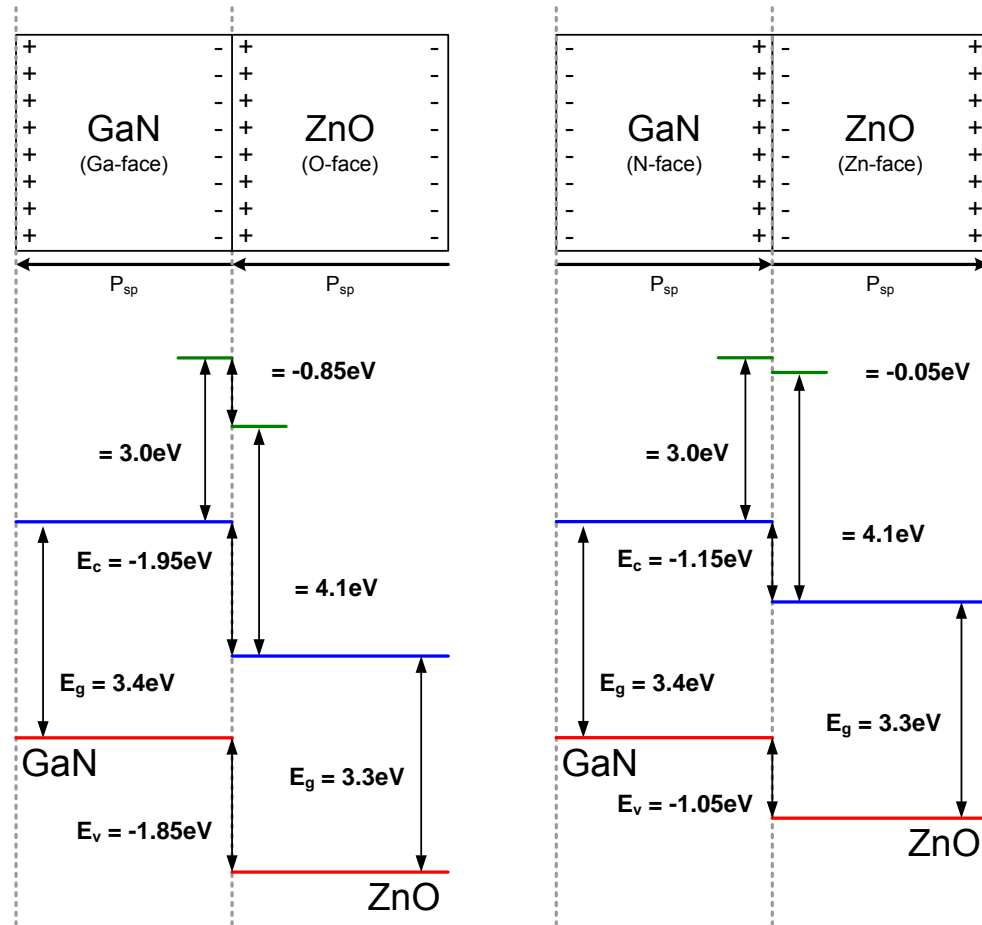
* W. Mönch, Universität Duisburg-Essen

Suggested Interface Structure



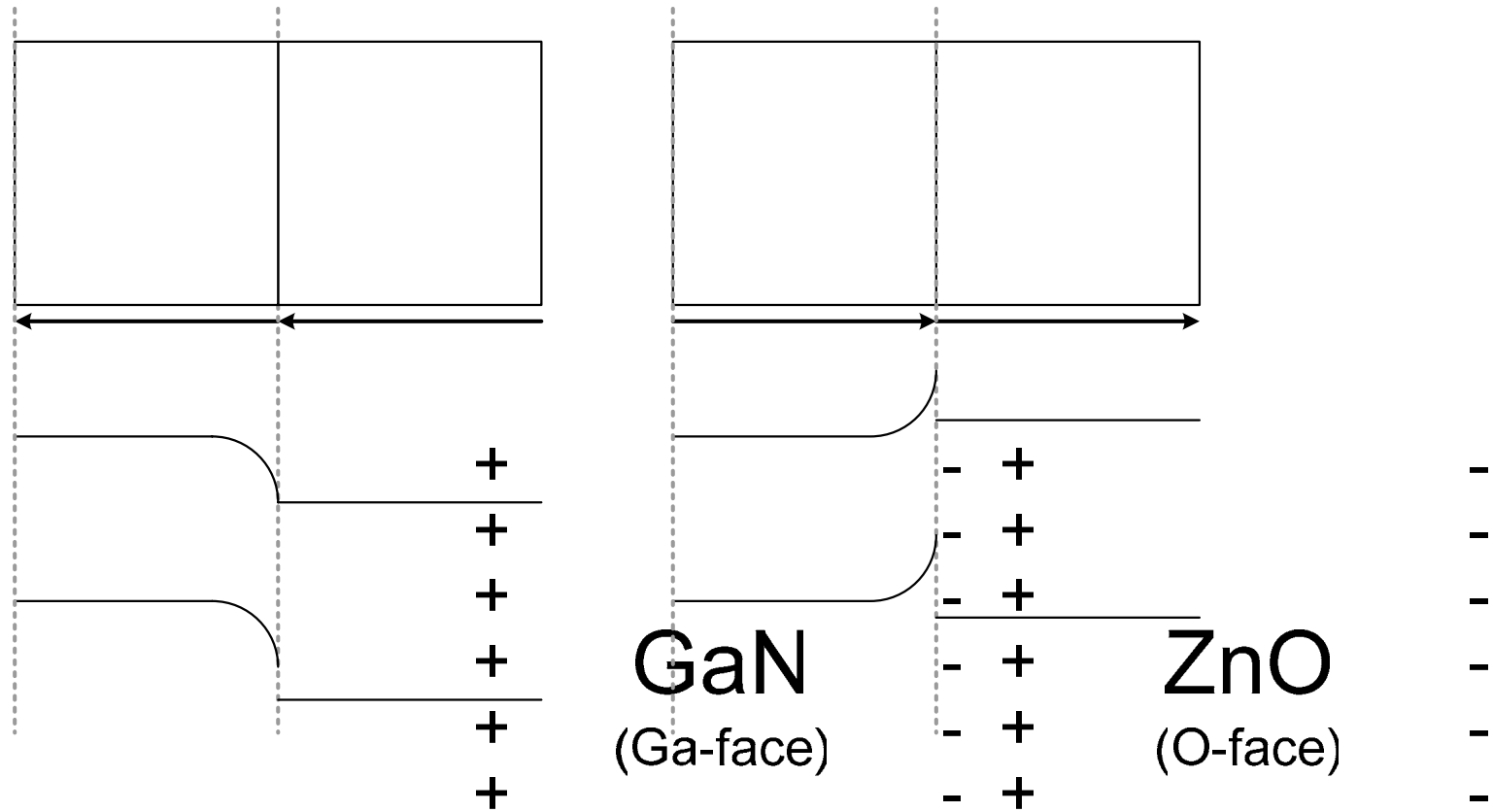
- GaN and ZnO are both polar materials
- Expect spontaneous polarization to align across the interface
- Direction of interface dipoles can increase or decrease barrier height

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?