

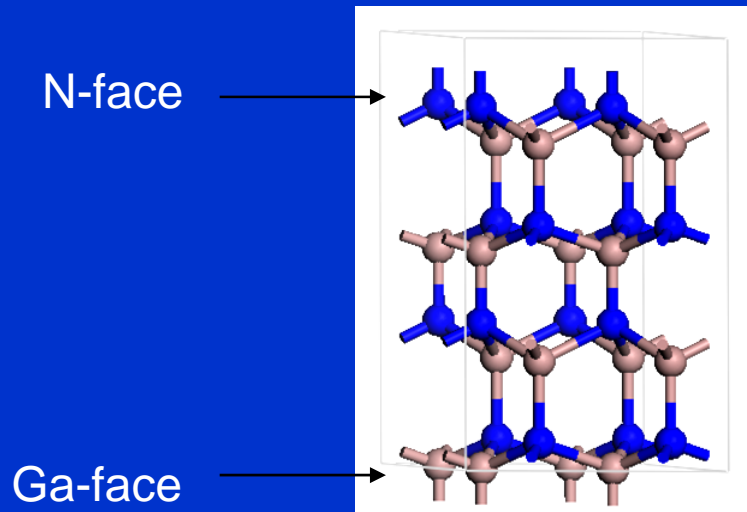
# *Structure and electronic properties of the polar ZnO-GaN (0001) interface*

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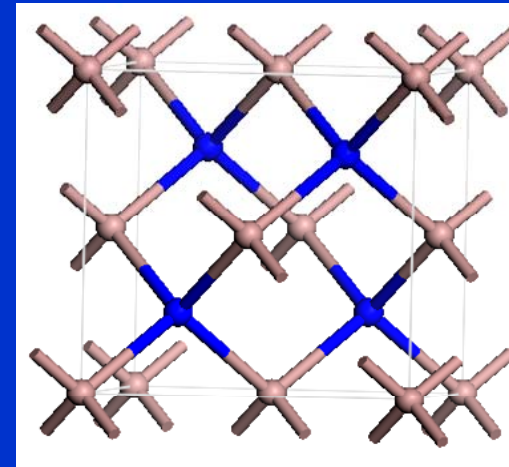
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# Properties of GaN

## Structure



wurtzite  
global minimum  
 $a, b = 3.189 \text{ \AA}$   
 $c = 5.185 \text{ \AA}$



zincblende  
Metastable  
 $a = 4.52 \text{ \AA}$

- Both zincblende and wurtzite material important
- Note polarity of wurtzite GaN along (0001) direction

# *Properties of GaN*

## Electronic Properties

- Large **direct band gap** of 3.44 eV that can be tailored to anything between 1.9 eV (650 nm) and 6.2 eV (200 nm) by alloying with In and Al respectively. Entire visible spectrum can be covered.
- Ideal for optoelectronic devices
- high breakdown field of  $3 \times 10^6 \text{ V cm}^{-1}$  – allows for high power operation
- high RT electron mobility of  $1350 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$

## Other important Properties

- strongly bonded with bond energies of 2.5 eV; reflected in **high melting point** ( $> 2500 \text{ K}$ )
- both n- and p-type material available

# *Applications of GaN*

## Optoelectronic Devices

- **Light Emitting diodes** in green/blue region of spectrum.
  - no viable alternative to GaN
  - traffic lights, energy-saving domestic lighting
  - LED-based white lighting by colour mixing (red, blue, green)
- **Laser diodes** - high frequency
  - High density optical storage devices
  - Predicted 4-fold increase in amount of information storable on a disk.

## Other Applications

- **FETs** and **UV detectors**.

# Growth of GaN

## The need for heteroepitaxy

- Bulk growth of GaN extremely difficult due to high MP of GaN. Only viable method is HNPS (Ga melt at 1700 °C under 20,000 atm of N<sub>2</sub>).
- Limited to very small crystallites.
- Also electronic properties of crystallites rather poor.
- hence foreign substrates have to be used

## Substrates for GaN Epitaxy

- **Sapphire** • basal-lattice constant mismatch of ~20 %,
  - thermal expansion coefficient > GaN
  - dislocation density ~ 10<sup>10</sup> cm<sup>-2</sup>
- **SiC** • better lattice matched (3.1 %)
  - thermal expansion coefficient < GaN
  - expensive

## *Alternative Substrates for GaN epitaxy*

- Need lower dislocation densities for more sophisticated devices, operating at more extreme conditions of temperature, voltages and current densities.

### **Choice of substrate**

- Important substrate properties that have to be considered for growth of high quality epilayers
  - Structure and lattice constant,
  - Composition and reactivity,
  - Thermal and electrical properties.
- Many different materials have been tried, but no ideal substrate has been found so-far.

# *ZnO as a Substrate for GaN epitaxy*

## Properties – similar to GaN

- isomorphic; close match in lattice constant (1.8 %);
- S/C, large band gap  $\sim 3.3$  eV, applications in high frequency LEDs
- strongly bonded – high melting point (2248 K)
- bulk material available

## Experimentally

- high quality GaN has been grown on ZnO (and vice versa).
- Recently LEDs based on the the GaN/ZnO interface have been reported.

## Study Outline

- Study atomic and electronic structure of GaN/ZnO interface
- In particular effect of interfacial compensation on stability and electronic properties of the interface was considered.

## *Method*

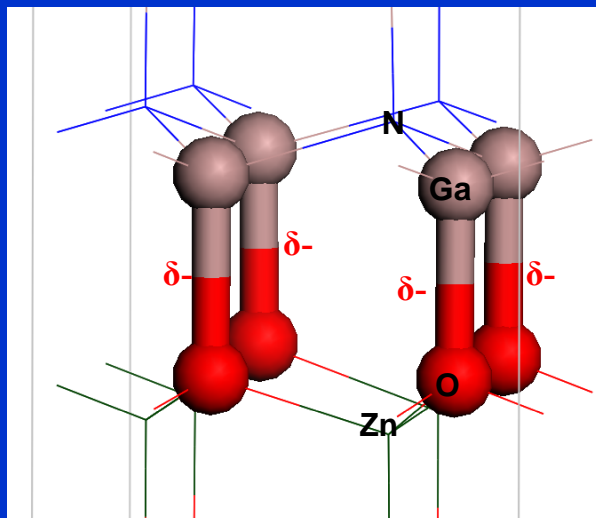
- PW DFT - CASTEP
- PBE functional – exchange correlation
- Periodic boundary conditions
- Ultrasoft Pseudopotentials to model ion-electron interaction



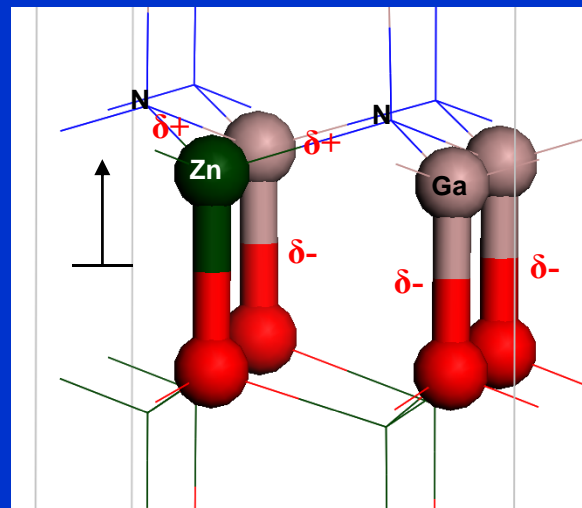
# The ZnO/GaN interface

## Heterovalent Interface

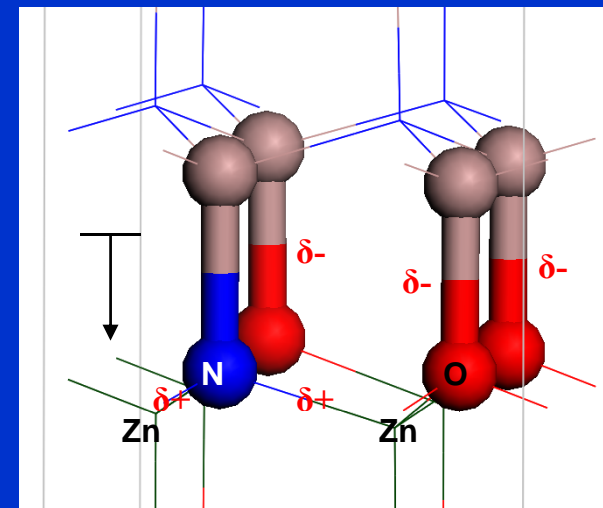
- considering cation/anion interfaces only, got Ga-O and Zn-N interfaces
- Abrupt Ga-O interface will contain an excess of  $\frac{1}{4}$  of an electron/bond; Zn-N interface will be deficient by  $\frac{1}{4}$  of an electron/bond  $\rightarrow$  substantial electric fields, destabilising interface.
- charge build-up can only be avoided by **atomic mixing** of interfacial layers, such that number of electron-rich bonds equal to electron deficient bonds
- opposite directions of **dipoles** for cation and anion compensation



abrupt



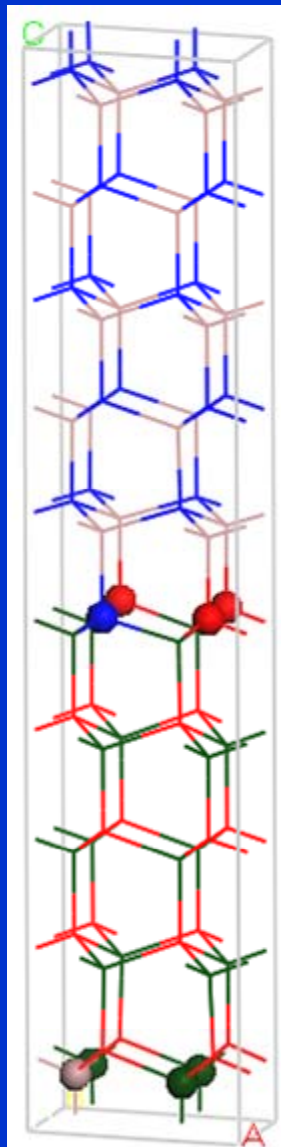
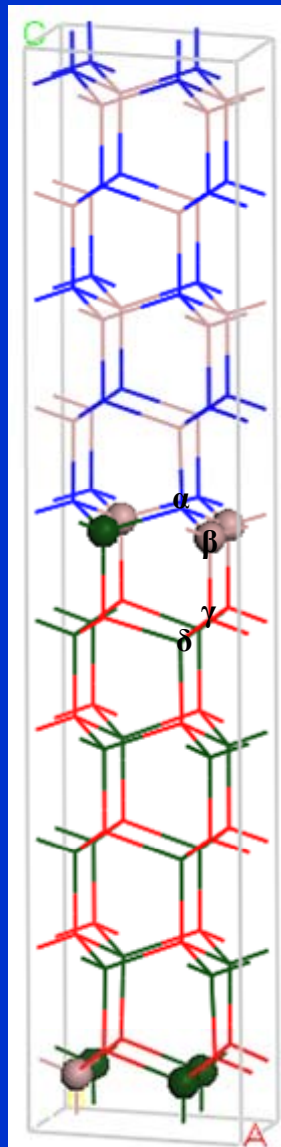
Zn-compensated



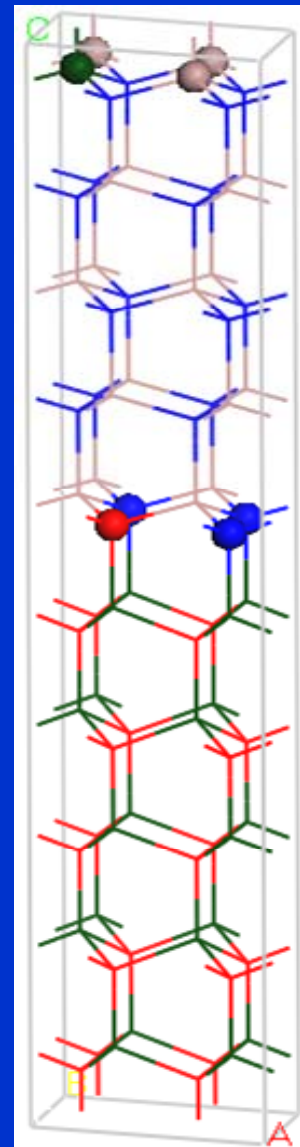
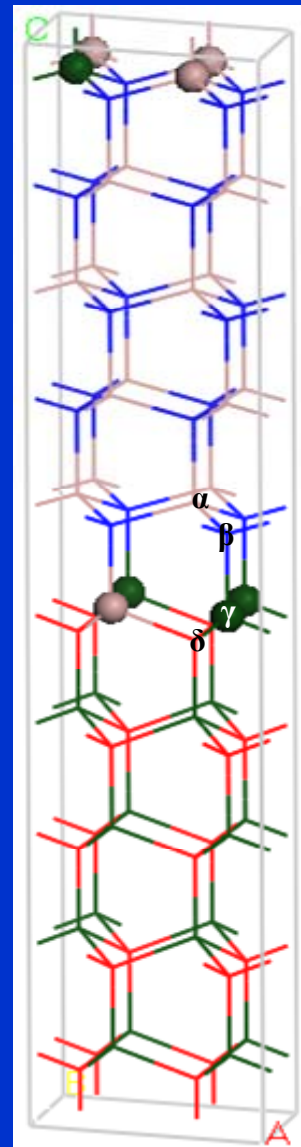
N-compensated

# *Interfaces Considered*

Ga-O interface



Zn-N interface



Reference Interface

Reference Interface

# Interfacial Formation Energy

- Interfacial formation energy defined as

$$E_f^{\text{int}} = \frac{1}{2} (E^{\text{tot}} - n^{\text{GaN}} \mu^{\text{GaN}} - n^{\text{ZnO}} \mu^{\text{ZnO}})$$

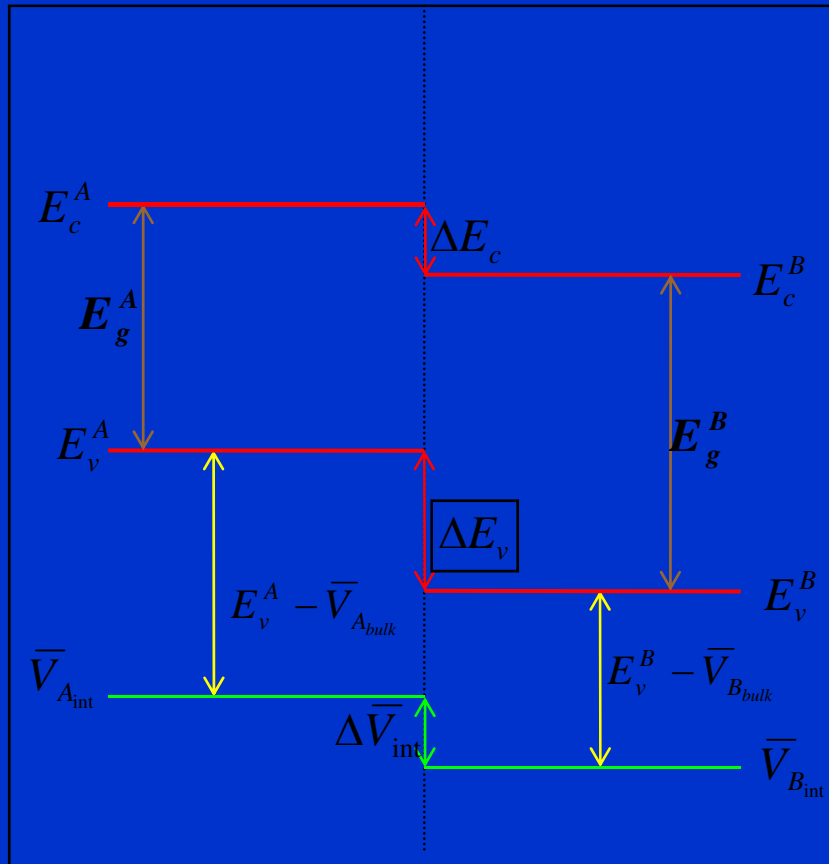
- two interfaces are not identical  $\rightarrow$  cannot derive *absolute* stability of different interfaces
- by introducing reference interface can determine relative stabilities of various interfaces of same polarity; i.e relative stability of 4 different Ga-O interfaces and relative stability of 4 different Zn-N interfaces, using

$$\Delta E_f^{\text{int}} = E_f^{SL_1} - E_f^{SL_2}$$

where

$$E_f^{SL_x} = (E_x^{\text{tot}} - n_x^{\text{GaN}} \mu^{\text{GaN}} - n_x^{\text{ZnO}} \mu^{\text{ZnO}})$$

# Determining the Valence band off set



Align

Bulk band structure of ZnO and GaN

to

average electrostatic potential of semiconductor slabs in supercell containing the interface

$$\Delta E_v = \Delta \bar{V}_{int} + (E_v^A - \bar{V}_{A_{bulk}}) - (E_v^B - \bar{V}_{B_{bulk}})$$

## *Results*

- Compensated interfaces are about twice as stable as non-compensated interfaces
- Cation-compensated interfaces are by about 15 meV more stable than corresponding anion-compensated interfaces
- Position of interface in wurtzite cell does not significantly affect its formation energy
- The valence band offset at the cation- and anion-compensated interfaces were found to be 1.0 eV and 0.5 eV, respectively.

## *Further Work on the ZnO/GaN interface*

Consider strain effects – used average basal lattice constant of GaN and ZnO so-far. Due to large piezoelectric constant of GaN and ZnO, expect dependence on strain state of heterojunction system. Rerun calculations using basal lattice constant of GaN and ZnO.

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