

# Atomistic Modeling of Nitride Devices

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## Why GaN/InN/GaN?

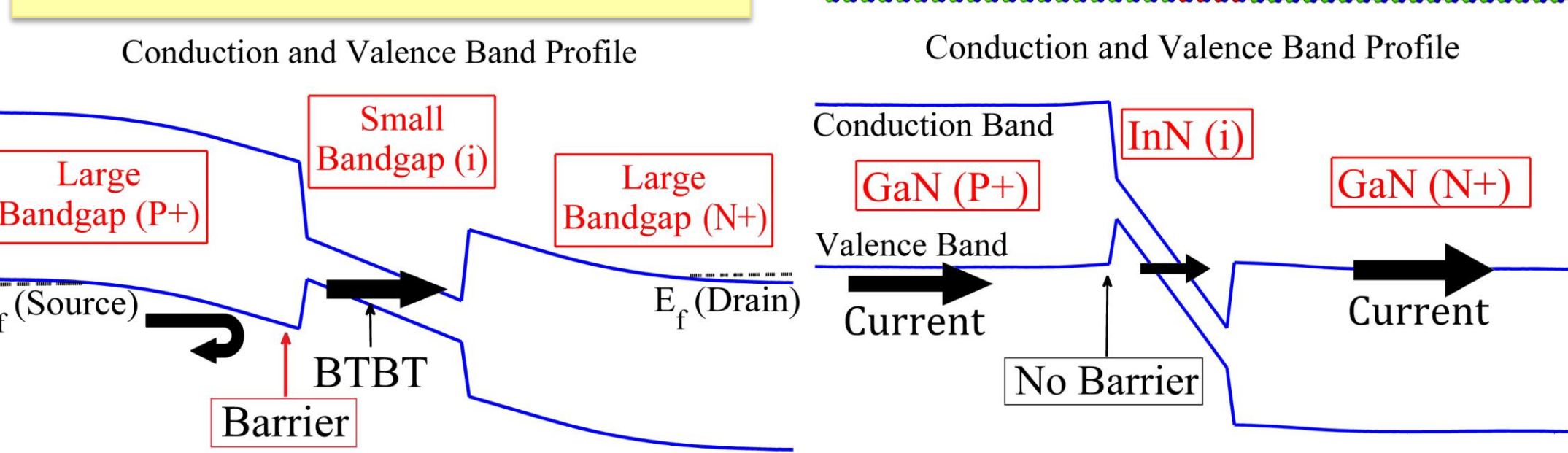
## Atomistic Tight Binding Simulation of Nitrides:

## Tight binding band-structure of InN and GaN

### Why GaN/InN/GaN is a good candidate for Tunnel FET?

1. Large internal electric field
  - Large band-bending over small distance
2. Small band gap InN
3. Both GaN and InN are direct Band-Gaps (BG)
  - Tunneling through direct BG is more than indirect ones

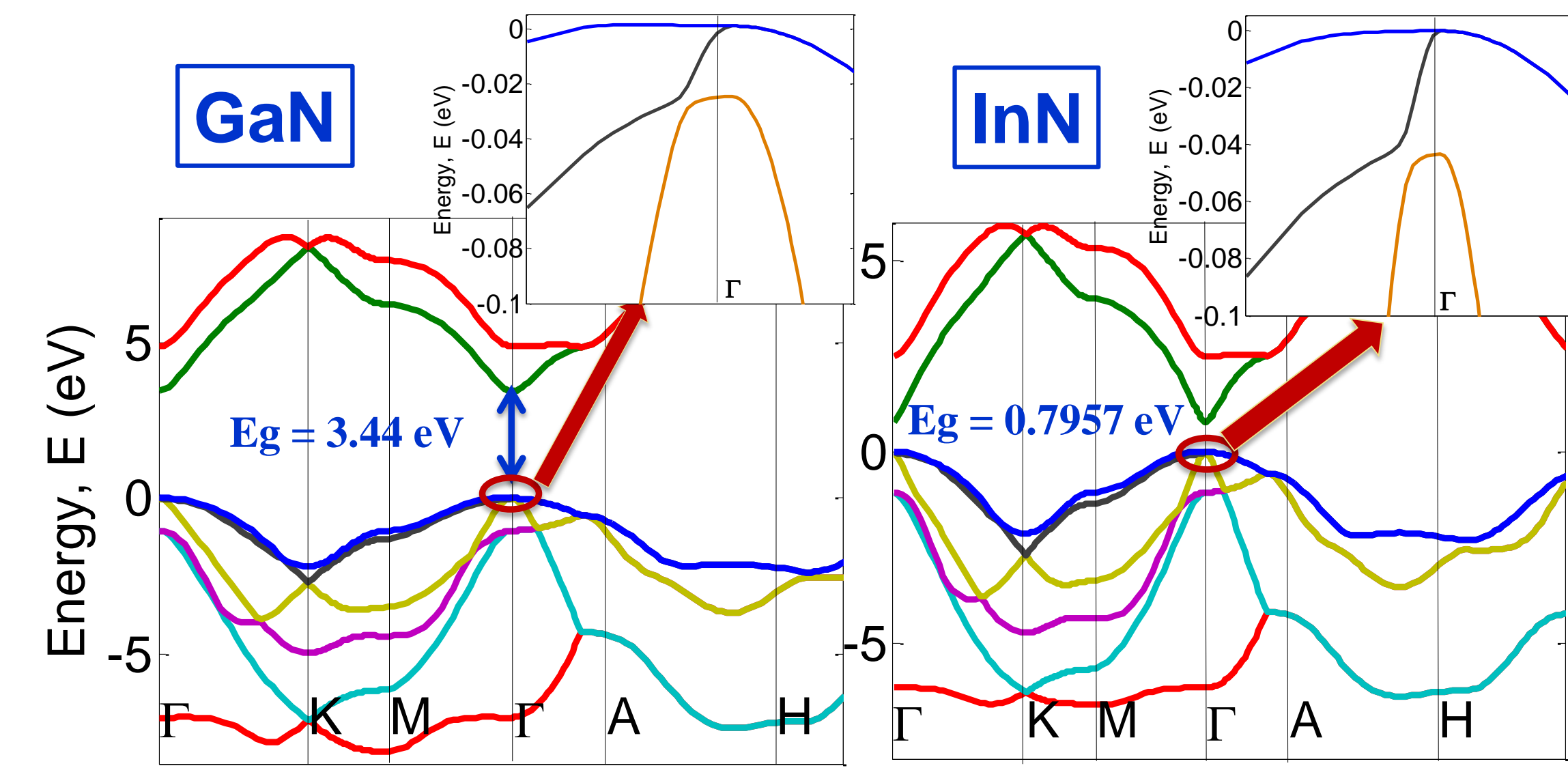
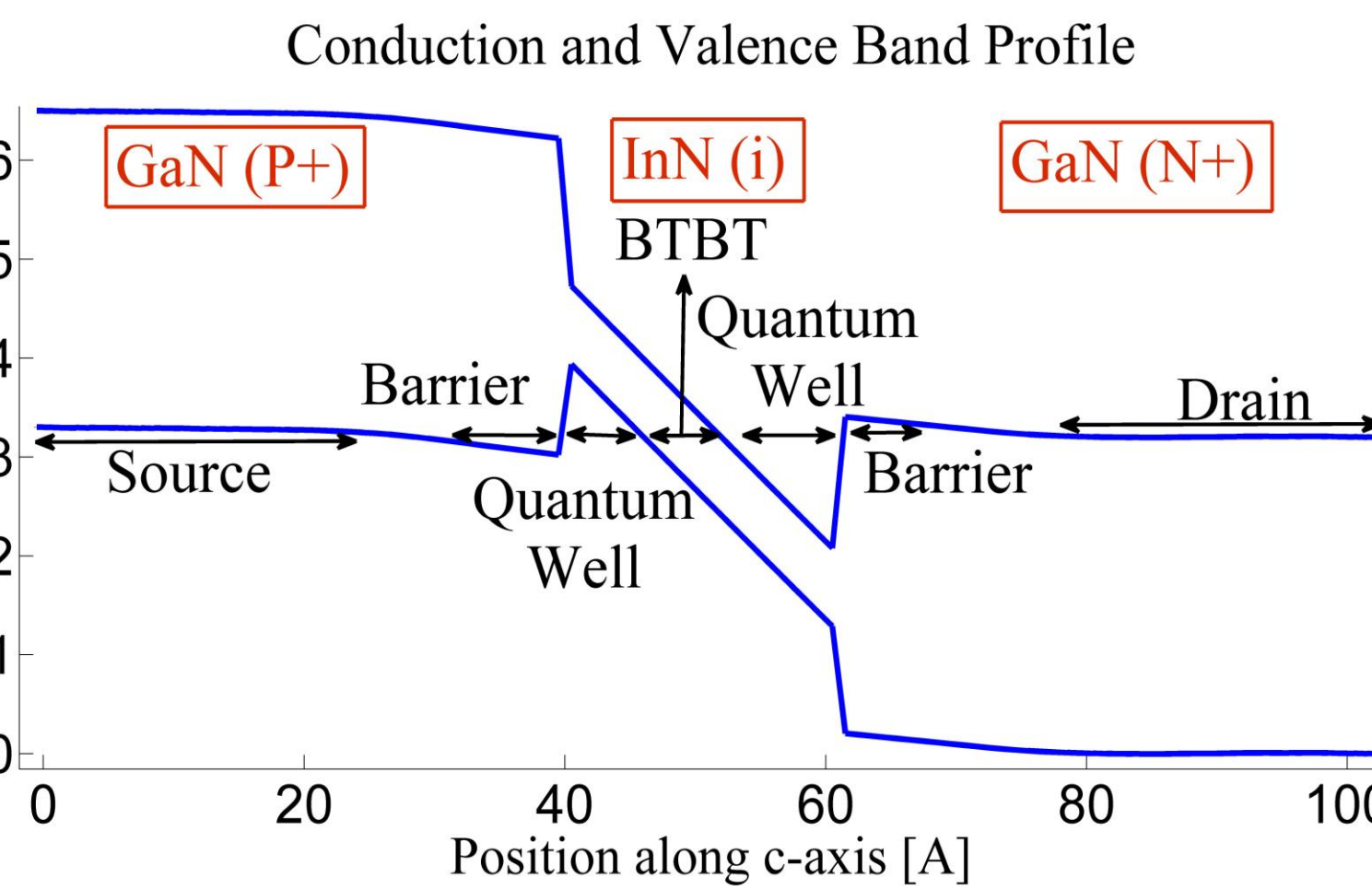
### Conventional hetero-structures



### Atomistic Tight-Binding simulation of Nitride TFET

It is Not just Band To Band Tunneling (BTBT)

1. Barriers may appear near source and drain
2. Quantum wells and BTBT region in InN



Atomistic tight binding captures the effects of

- Crystal-field splitting
- Spin-orbit coupling

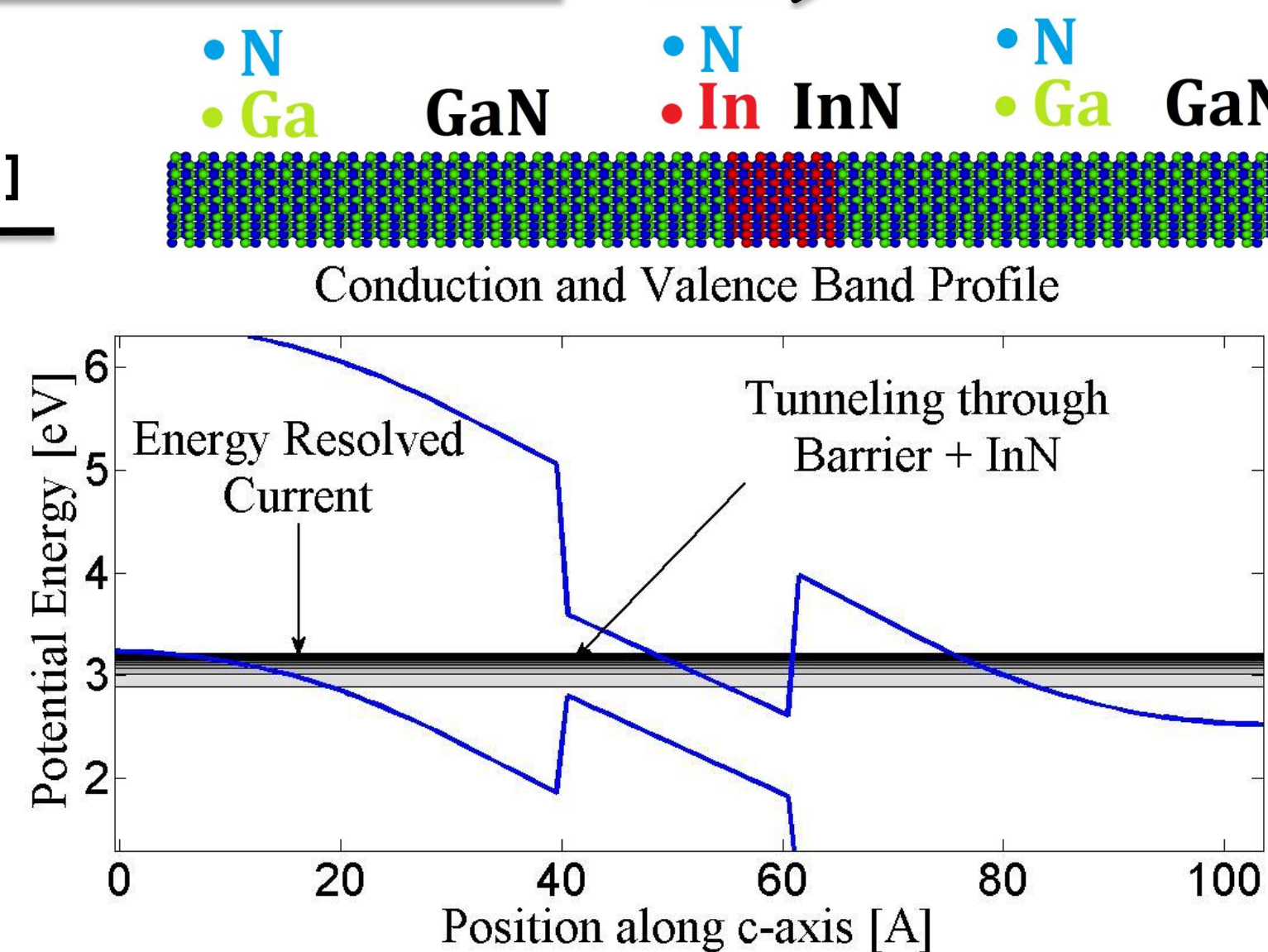
## Ga-Face Growth

### 2nm Long InN (Ga-Face Growth)

- 1) Pyro field is against built-in PN junction field
- 2) The electric field is not large enough to make band bending
- 3) Tunneling magnitude is very small

### PN Junction Built in field

Pyro



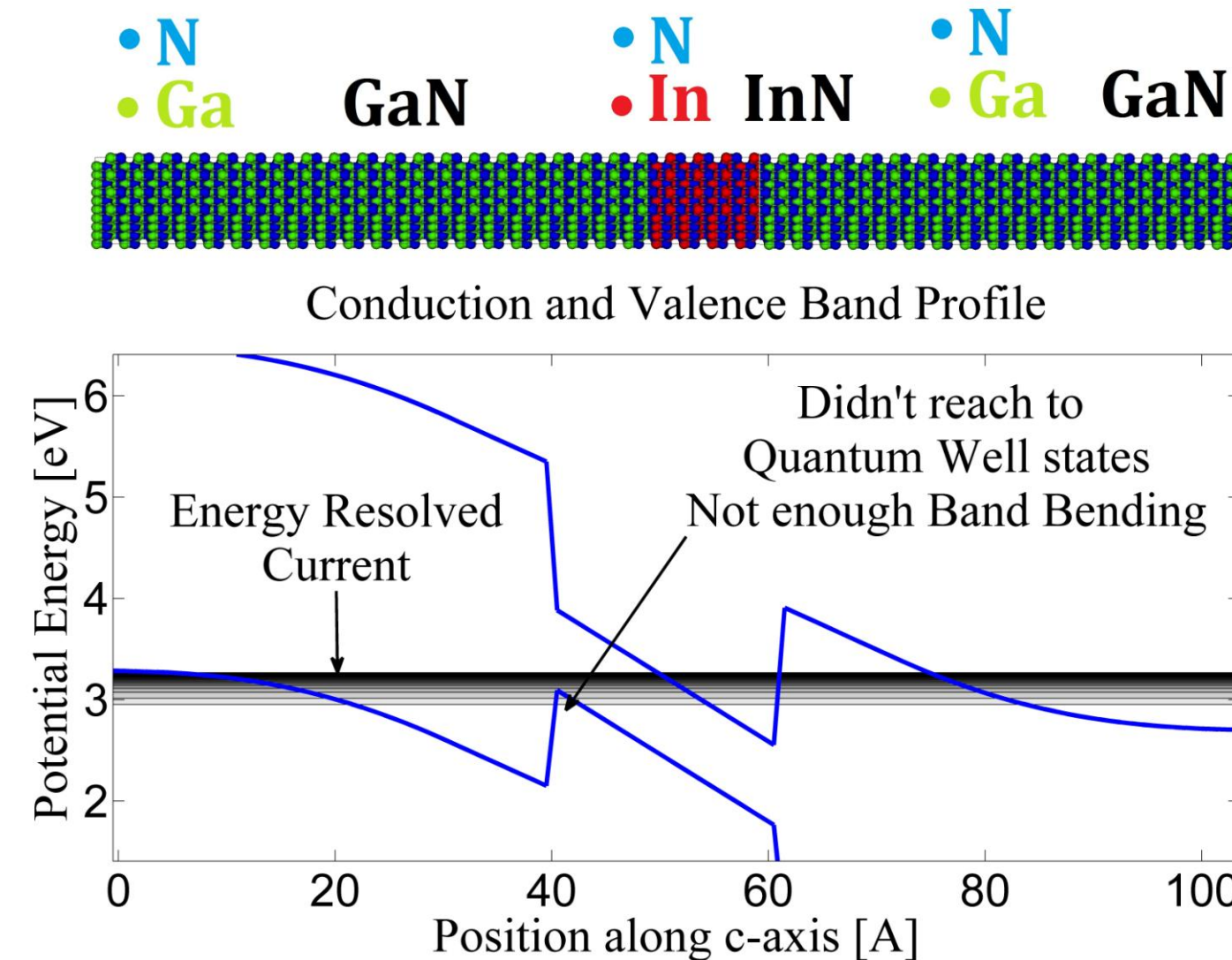
## N-Face Growth

### 2nm Long InN (N-Face Growth)

- 1) Pyro field adds up to built-in PN junction field
- 2) The electric field is not large enough to make band bending
- 3) Tunneling magnitude is larger but not significantly

### PN Junction Built in field

Pyro



## Piezoelectric effect

### Piezoelectric effect (Parameters [1])

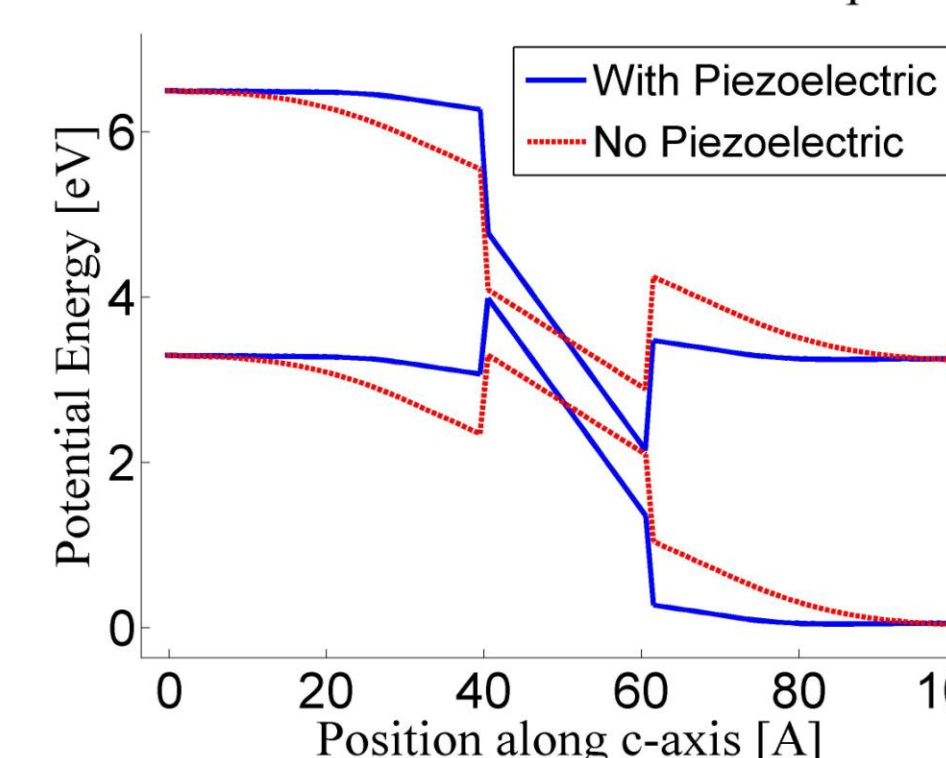
- 1) E(Piezo) ~ 15 x E(Pyro) in InN
- 2) E(Piezo) is larger than 1V/nm
- 3) Huge band bending

[1] J. Phys.: Condens. Matter 14 (2002) 3399-3434

### Parameters:

- 1) P(Piezo) = 0.15 C/m^2
- 2) 1.5nm InN thickness

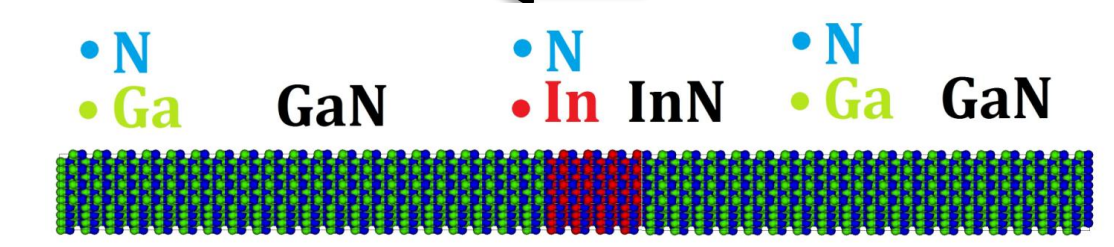
### Conduction and Valence Band profile



### Piezoelectric

PN Junction Built in field

Pyro



## Piezoelectric effect

### Piezoelectric effect (Parameters [2])

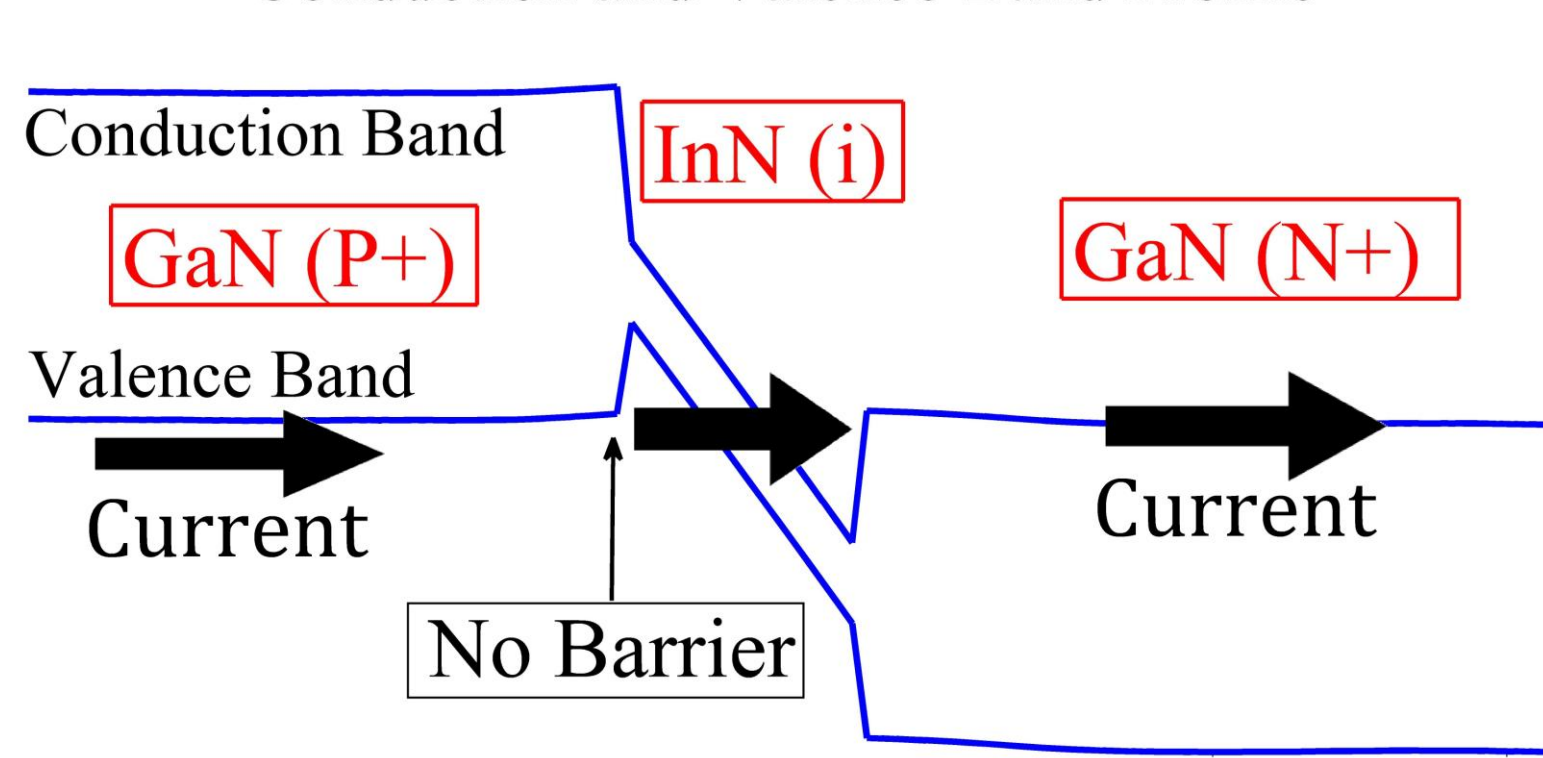
- 1) No barrier to reach BTBT region
- 2) E(Piezo) ~ 25 x E(Pyro) in InN
- 3) E(Piezo) is larger than 2V/nm

[2] Phys. Rev. B 56 (1997), R10024-R10027

### Parameters:

- 1) P(Piezo) = 0.25 C/m^2
- 2) 1.5nm InN thickness

### Conduction and Valence Band Profile



## Output characteristics

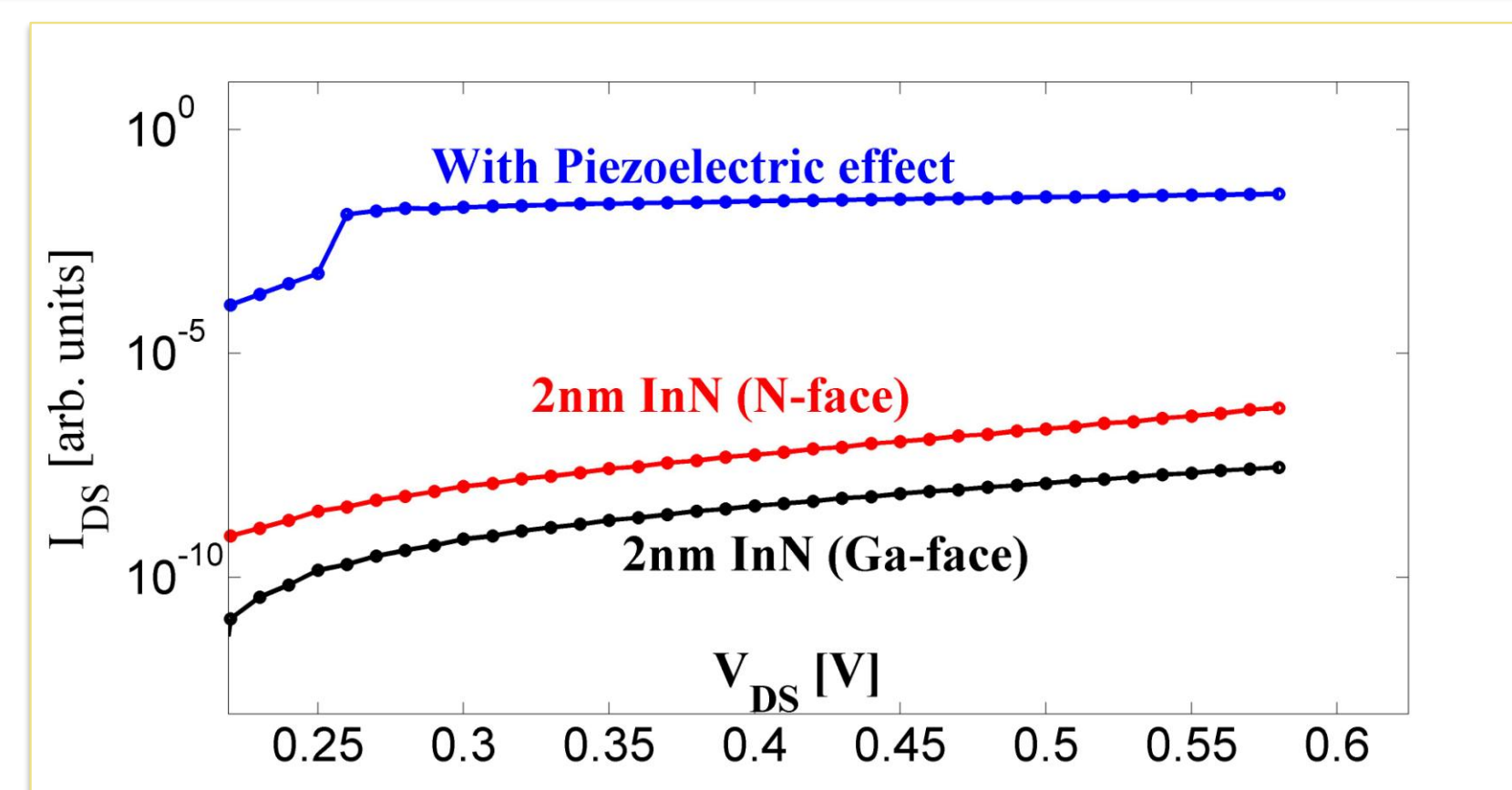
### The device structure needs to be engineered

Goal: tunneling through the low gap region

Problem: barriers to reach to the low gap region

Solution: piezoelectric effect can lower the barriers down to zero

Piezoelectric effect has the most important impact on the performance



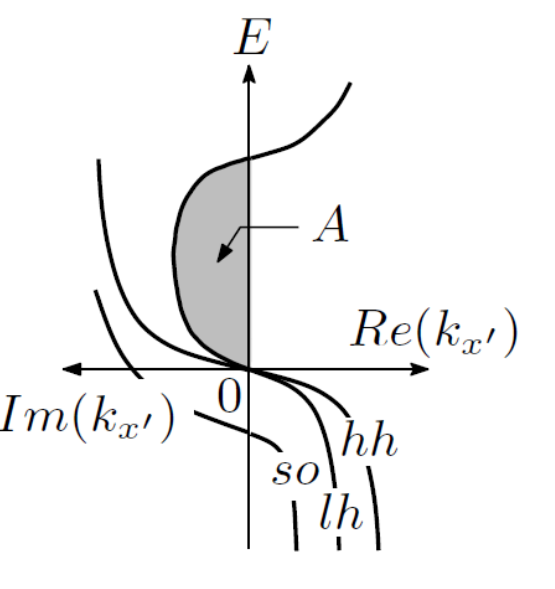
## InN complex band-structure

Most probable BTBT minimizes the area  $A = \int_{E_v}^{E_c} \text{Im}\{K\} dE$

$$\text{BTBT Probability } T = e^{-\frac{2A}{qF}}$$

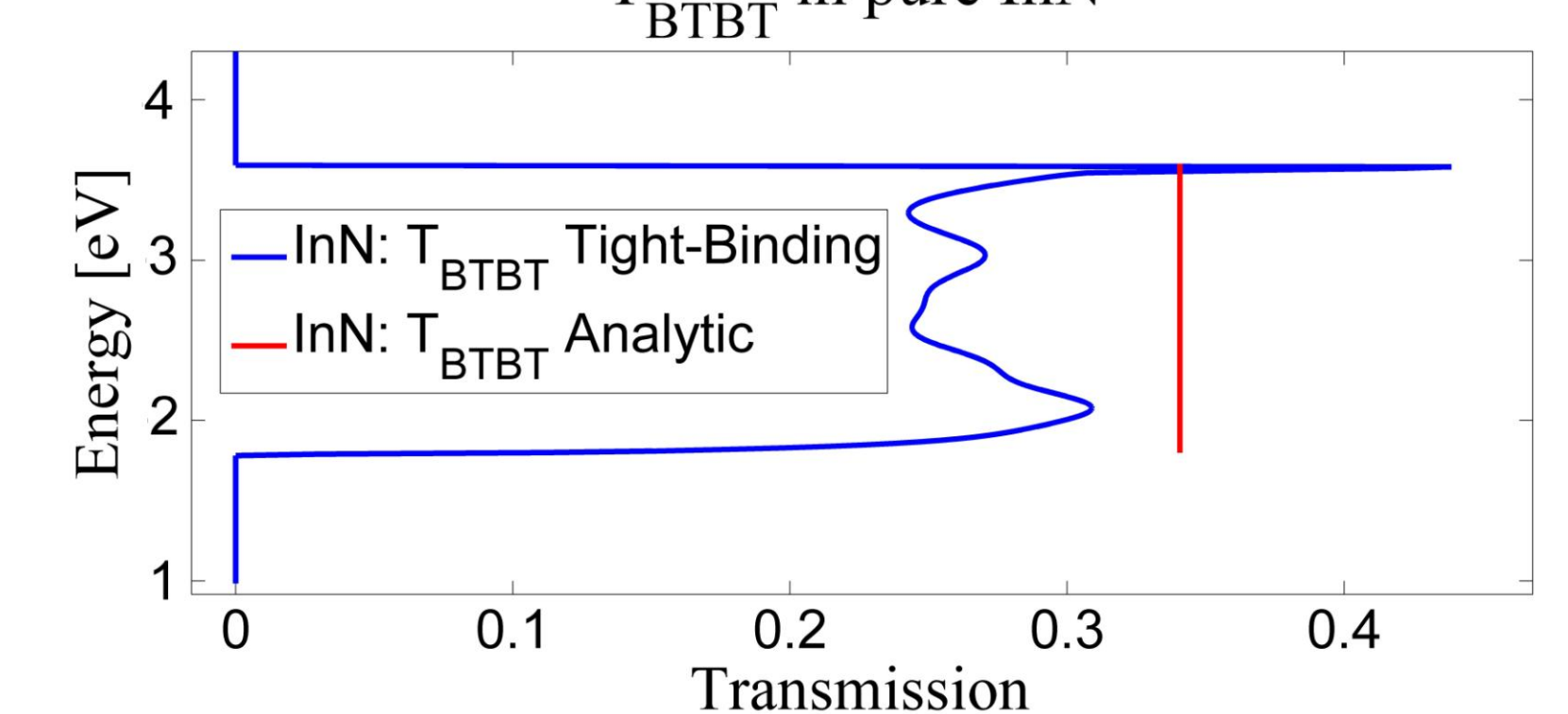
F = Electric field in depletion region

$$\text{For pure InN, } T_{\text{BTBT}} = e^{-\frac{0.07}{F}}, F = \text{E-field (V/\AA)}$$



from Arvind Ajay's PhD Thesis

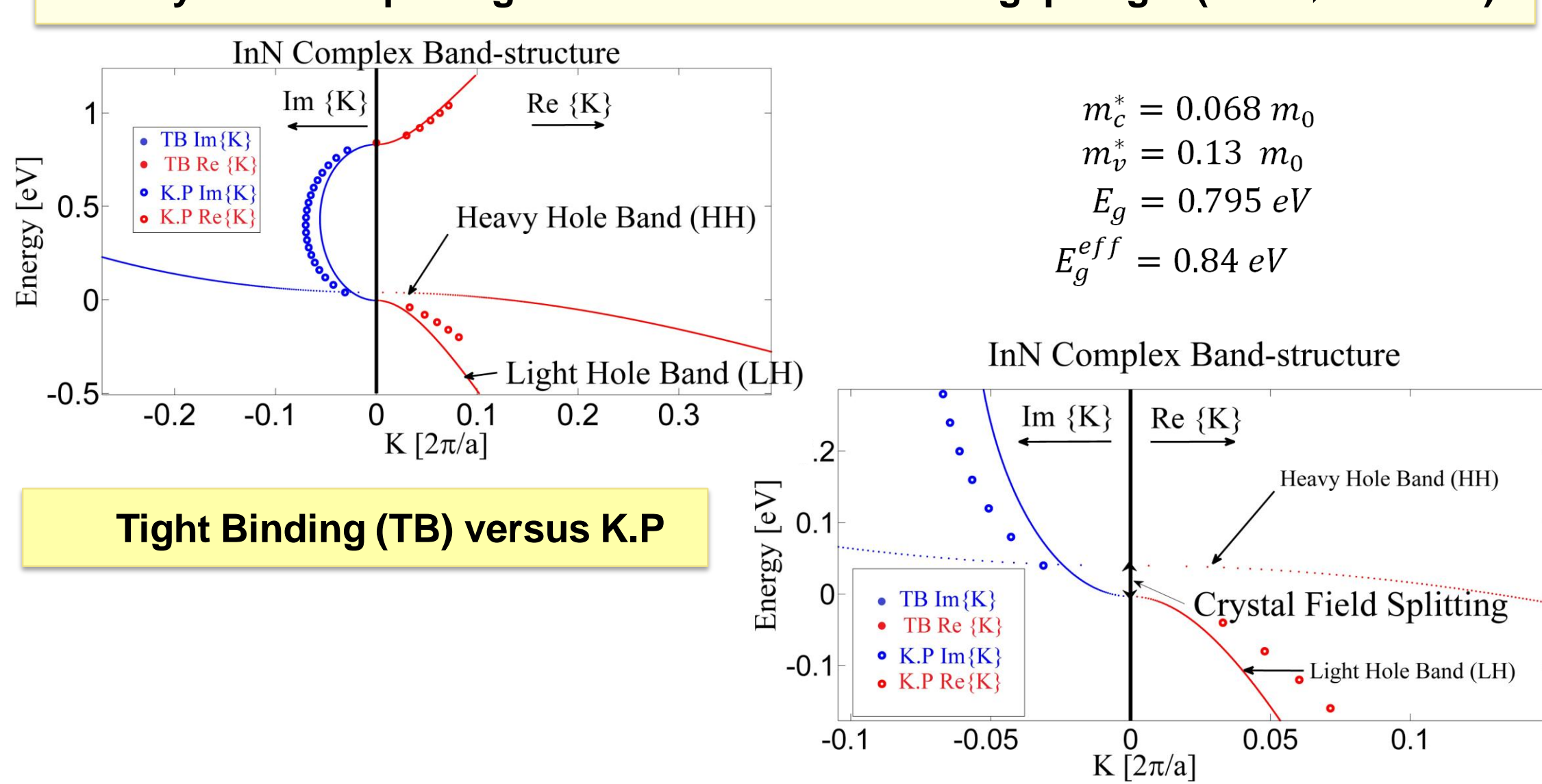
### T<sub>BTBT</sub> in pure InN



## Complex Band Structure of InN

- Heavy Hole and Light Hole band splits due to crystal field splitting
- Light Hole band plays important role (minimum area A)

### Crystal field splitting makes the effective band-gap larger (0.79→ 0.84 eV)



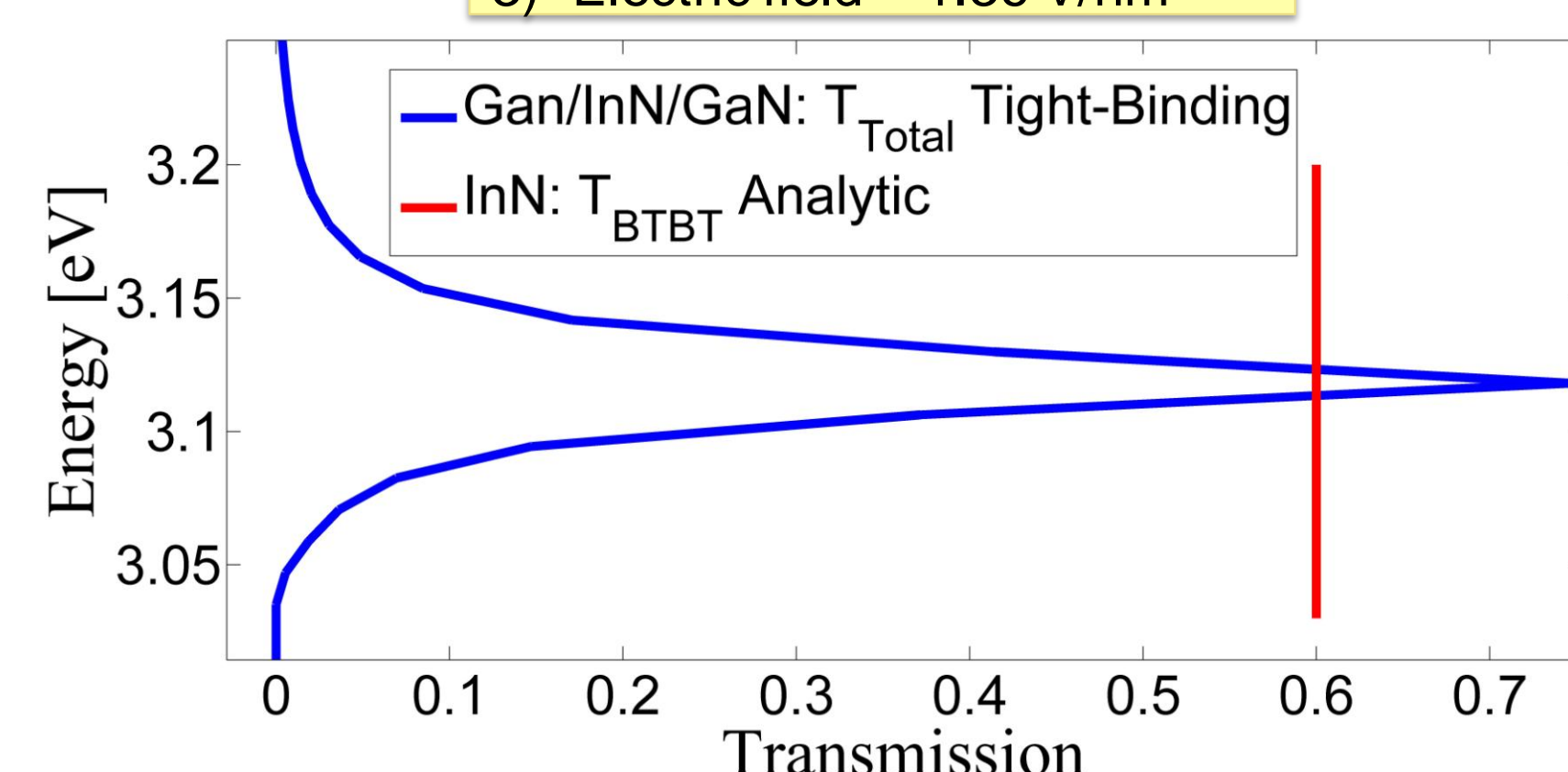
## Band To Band Tunneling Probability in GaN/InN/GaN

### Tunneling probability in GaN/InN/GaN is not much lower than InN

### Small reduction in Transmission due to Barriers

### Parameters:

- 1) P(Piezo) = 0.15 C/m^2
- 2) 2.0nm InN thickness
- 3) Electric field ~ 1.36 V/nm



## Conclusion

### Using self consistent Poisson-NEGF\*, we studied GaN/InN/GaN

- The effect of Ga-Face and N-Face growth on the band profile was analyzed
- The piezoelectric effect studied with 2 different parameter sets
- Complex band structure of InN calculated using Tight Binding and K dot P
- Simple analytic equation for Band To Band Tunneling through InN devised
- The analytic equation verified against numerical simulation

GaN/InN/GaN is shown to be a good candidate for Tunnel FETs

\*NEGF: Non-Equilibrium Greens Function