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Interfacial Trap Effects in InAs Gate-all-around Nanowire Tunnel Field-Effect Transistors: First-Principles-Based Approach

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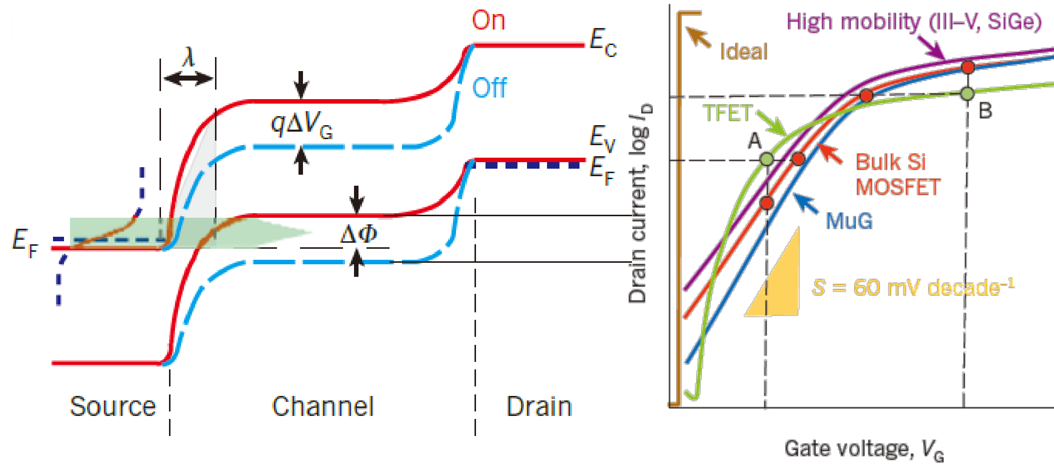
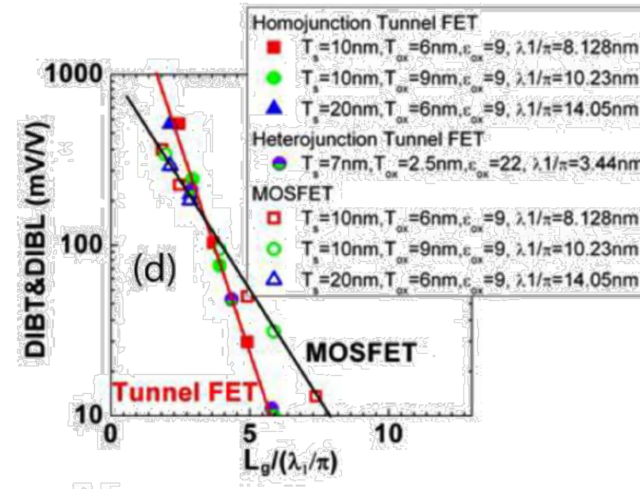
Outline of Presentation

- Motivation
  - Single defect effect
- Simulation approach
  - DFT defect modeling / NEGF
- Simultaion result
  - L_G scaling / x_T variation
- Conclusions

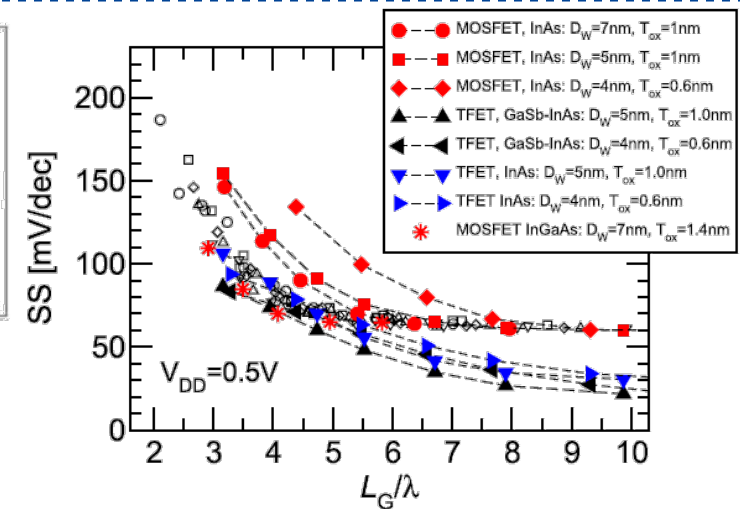
Motivation Potential of TFET



A. M. Ionescu et al., *Nature*, 2011

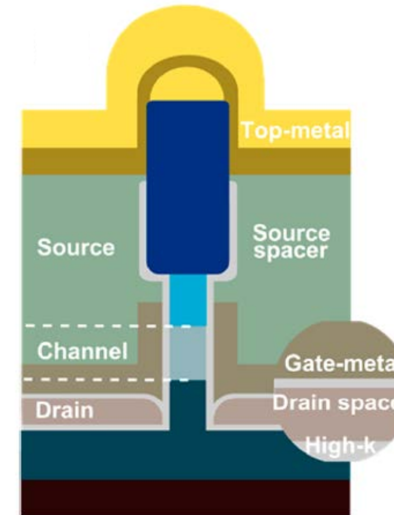


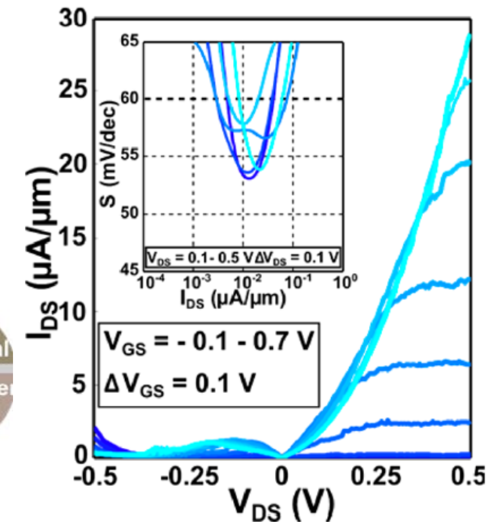
L Liu et al., *IEEE TED*, 2012



D. Esseni et al., *IEEE TED*, 2015

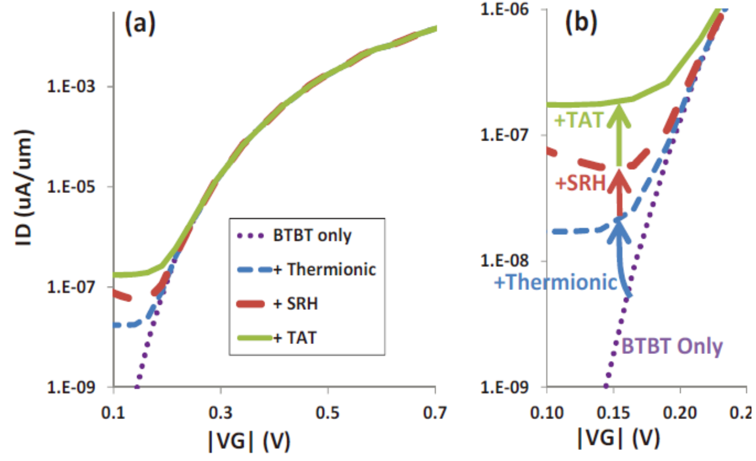
- **Low OFF-state current**
- **Band-to-band tunneling → SS < 60 mV/dec**
- **Good scalability**
- **Low ON-state current issue**
  - ✓ **Heterojunction (III-V/III-V, III-V/Si)**
  - ✓ **Gate-all-around nanowire (GAA NW)**

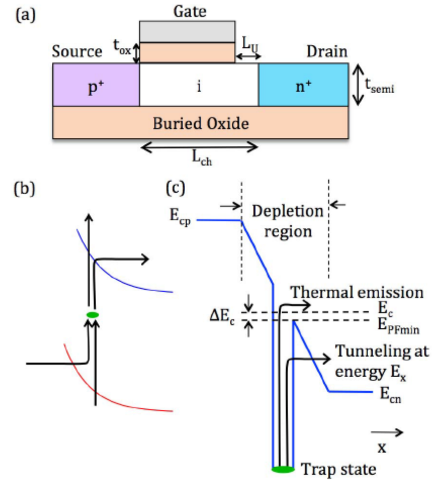




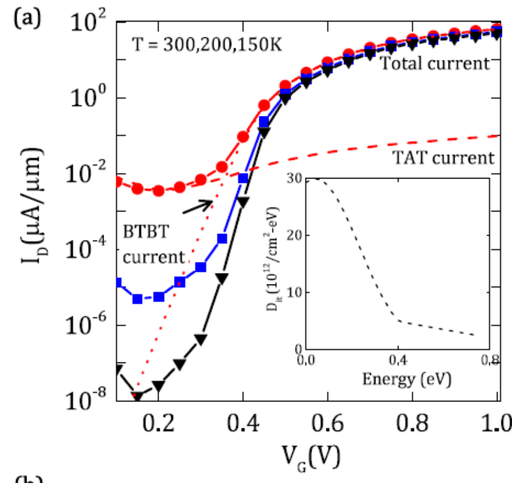
E. Memsievic et al., *Nano Lett.*, 2017

Defect-induced degradation

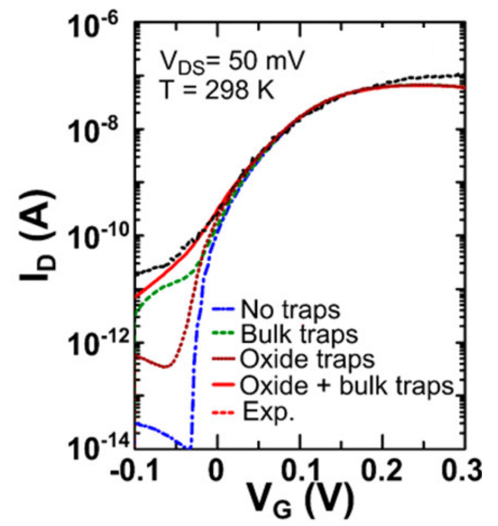




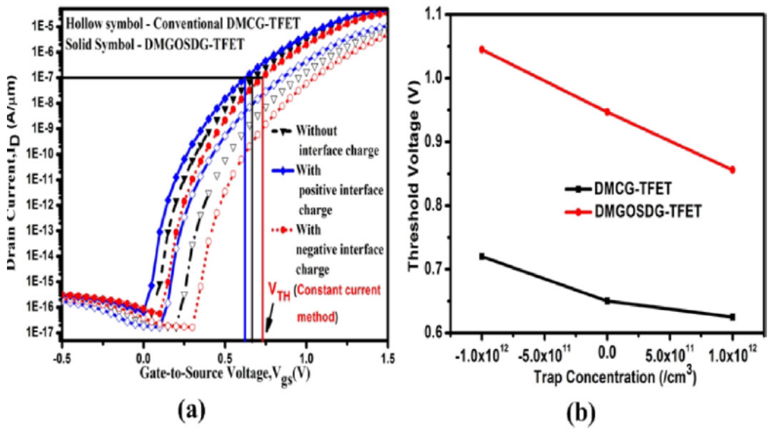
U. E. Avci et al., *IEDM*, 2015



R. N. Sajjad et al., *IEEE TED*, 2016



E. Memsievic et al., *Nano Lett.*, 2017



Km. S. Singh, et al., *IEEE T. Device Mat. Re.*, 2020

Defect has been one of the critical issue for the practical applications of TFETs

- **Trap-assisted tunneling (TAT)**
- **Electrostatic degradation by trapped charges**

Low-defect fabrication process of NW

→ Importance of a single defect analysis on GAA NW III-V TFET at nanoscale

Defect models – previous works

Conventional TCAD model

- Many fitting parameters for various current mecahnisms (BTBT, TAT)
- Limit of the analysis of the impact of a single defect on NW TFET at nanoscale

Full quantum transport model for a single defect is necessary

Nonequilibrium Green's function (NEGF) studies for a single defect

- $k \cdot p$ Hamiltonian + Cubic potential well (M. G. Pala, *IEEE TED*, 2013)
- Tight-binding (TB) Hamiltonian + Screened Coulomb potential (P. Long, *JAP*, 2018)
- TB Hamiltonian with adjusted TB parmeters (M. Rau, *Ph.D. Thesis*, 2019)

- Lack of physical defect information → No linkage between **specific defect types** and **TFET performances**
- Charge trapping effects have not been rigorously treated

→ **Physically-relevant atomic defect Hamiltonians are essential**

Contribution

In this work,

- ✓ Physically-relevant interfacial defects whose energy level is located in the band gap are handled by the first principles approach for InAs/Al_2O_3 GAA NW TFET
- ✓ Full quantum tranport model including electron-phonon scattering is employed to exactly capture the trap-assisted tunneling (TAT) and charge trapping in the defect states
- ✓ The impact of gate length (L_G) scaling with a single trap are closely investigated

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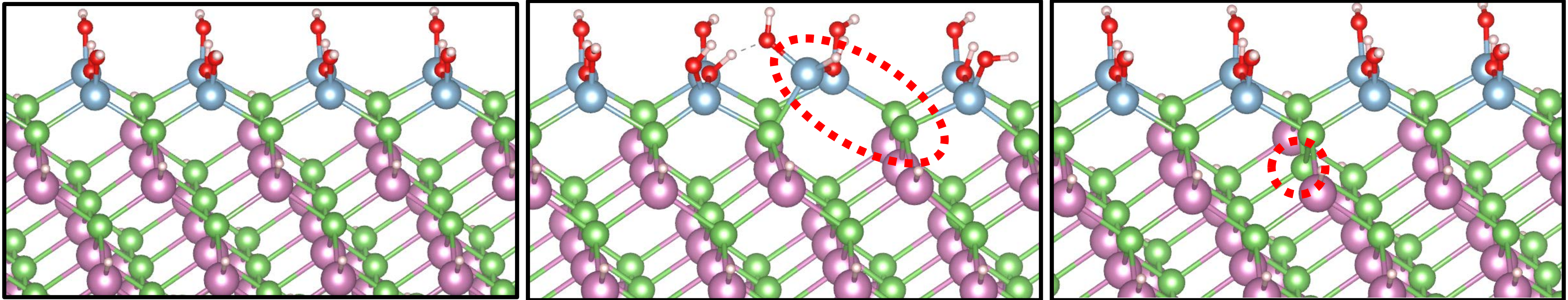
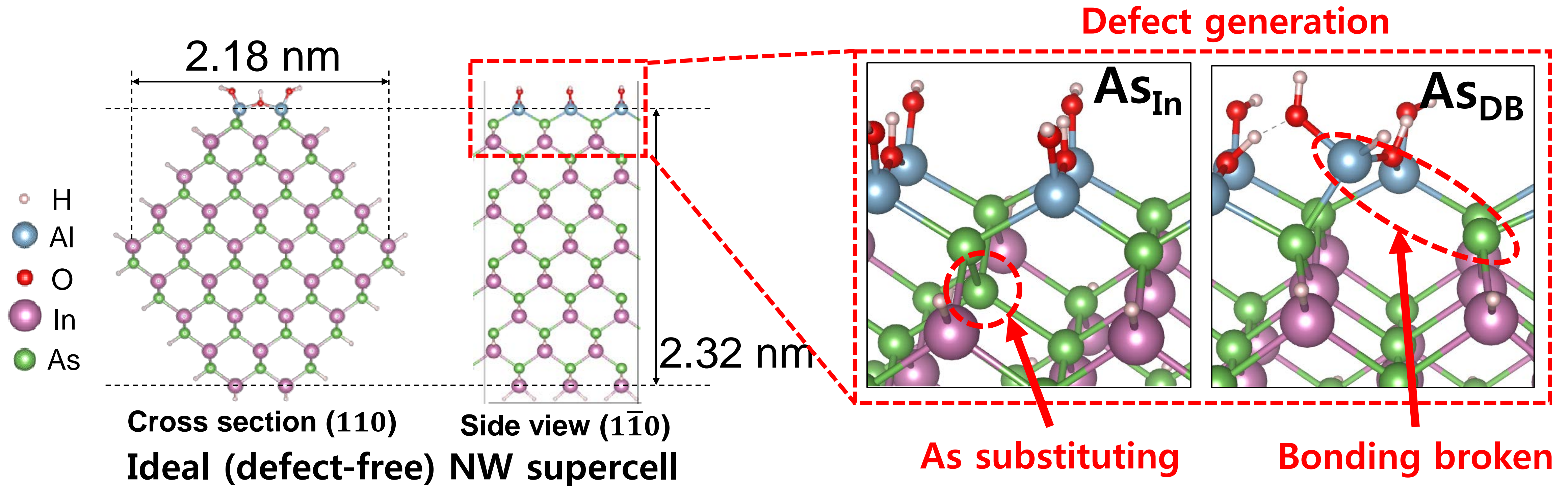
DFT defect modeling



- Several first-principles studies on the interfacial defects at III-V/high-k oxide have reported that **dangling bond** and **antisite** are dominant sources for **bandgap defect** [1], [2]
- In this work, **As-dangling bond (As_{DB})** and **As-antisite (As_{In})** between InAs/Al_2O_3 nanowire are considered

[1] J. Robertson et al., *JAP*, 2015 [2] G. G. Diniz et al., *JAP*, 2017

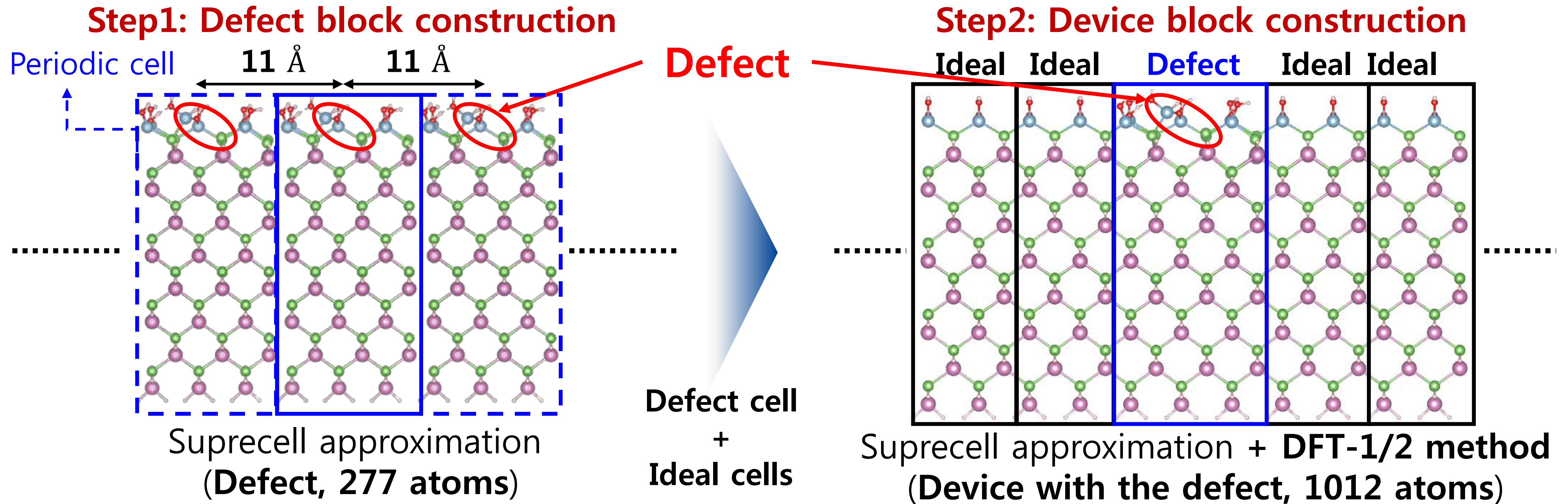
DFT defect modeling



- InAs/Al_2O_3 NW with 2.18 nm x 2.32 nm
- **DFT** in the basis of **LCAO** using the **SIESTA package**
- Exchange-correlation: **GGA-PBE** functional

[1] L. G. Ferreira et al., *PRB*, 2008 [2] L. Lin, *JAP*, 2013

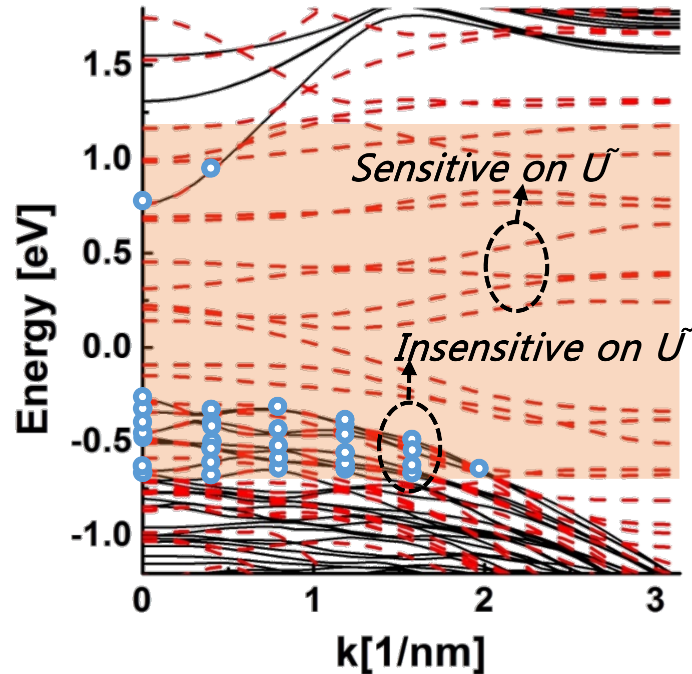
DFT defect modeling



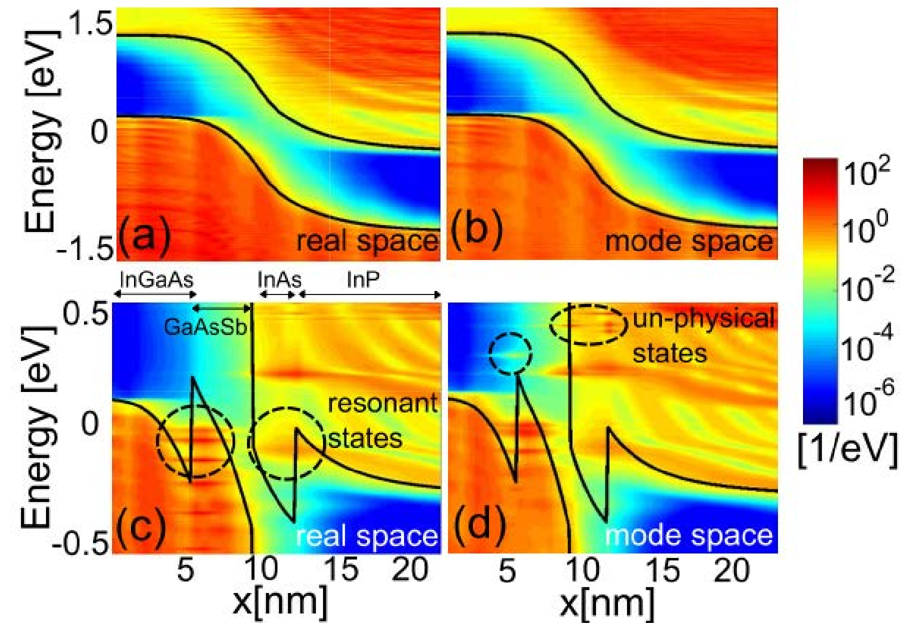
- Spacing between the periodic defects ≥ **11** Å to eliminate **the interaction between imaginary defects** [1]
- Bandgap underestimation of **GGA** is corrected by employing the **DFT-1/2 method** [2]
- Structure relaxed until maximum force < 0.05 eV/Å with 3x1x1 Monkhorst-Pack k-grids

[1] L. Lin, *JAP*, 2013 [2] L. G. Ferreira et al., *PRB*, 2008

Mode-space in heterostructures



[1] M. Shin et al., *JAP*, 2016



[2] C. Y. Chen, *IEEE TED*, 2020

- The size of DFT Hamiltonians is prohibitively large for the NEGF simulations
- **Mode space method** originally developed for DFT Hamiltonian [1] is extended to **heterogeneous system** where **a single defect** is introduced
  → Our novel method gurantees no unphysical states mentioned in [2]

NEGF Phonon scattering

Limit of ballistic NEGF simulation for defect study

- Defect density of states is very sharp (Dirac-like LDOS)
  → Convergence problem during self-consistent calculations between NEGF and Poisson's equations [1]
- Non-physical behavior, such as artificial negative differential resistance, may occur without inelastic scattering [2]

Electron-phonon scattering (**elastic/inelastic**) is included using deformation potential [3] within self-consistent Born approximation

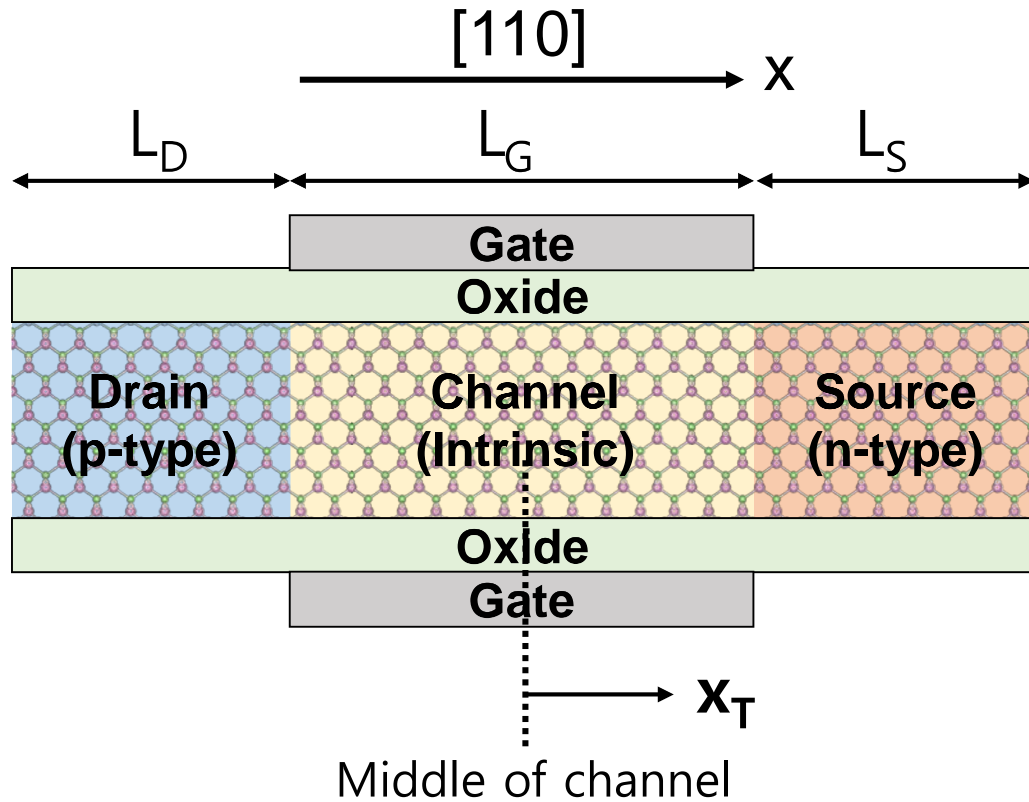
$$\boldsymbol{\Sigma}_{ac}^{\lessgtr}(E) = \frac{D_{ac}^2 k_B T}{\rho v_s \Omega} \boldsymbol{S}\boldsymbol{G}^{\lessgtr}(E)\boldsymbol{S}$$

$$\boldsymbol{\Sigma}_{op}^{\lessgtr}(E) = \frac{\hbar D_{op}^2}{2\rho\omega\Omega} \boldsymbol{S}\left(n_\omega \boldsymbol{G}^{\lessgtr}(E+\hbar\omega) + (n_\omega + 1)\boldsymbol{G}^{\lessgtr}(E-\hbar\omega)\right)\boldsymbol{S}$$

$D_{ac/op}$: acoustic/optical deformation potentials

[1] thesis, Rau, 2019
[2] M. Bescond, JAP, 2010
[3] C. Klinkert, ACS Nano, 2020

Simulation setup / parameters



Gate length (L_G) scaling simulation

L_G is varied from 7 nm to 17 nm
Defect is asummed to be located in the middle of the channel

Defect location (x_T) simulation

x_T is varied from -6 nm to 6 nm
- Drain-side defect ($x_T < 0$)
- Source-side defect ($x_T > 0$)

L_G is set to be 17 nm

V_{DD} : 0.4 V
I_{OFF} : 10 pA/μm
Doping density : 5×10^{19} cm^{-3}
EOT : 0.43 nm
L_D/L_S : 20 nm / 40 nm

D_{ac} : 5.8 eV (electron), 1.0 (hole)
D_{op} : 2.0 eV/A
$\hbar\omega$: 30 meV

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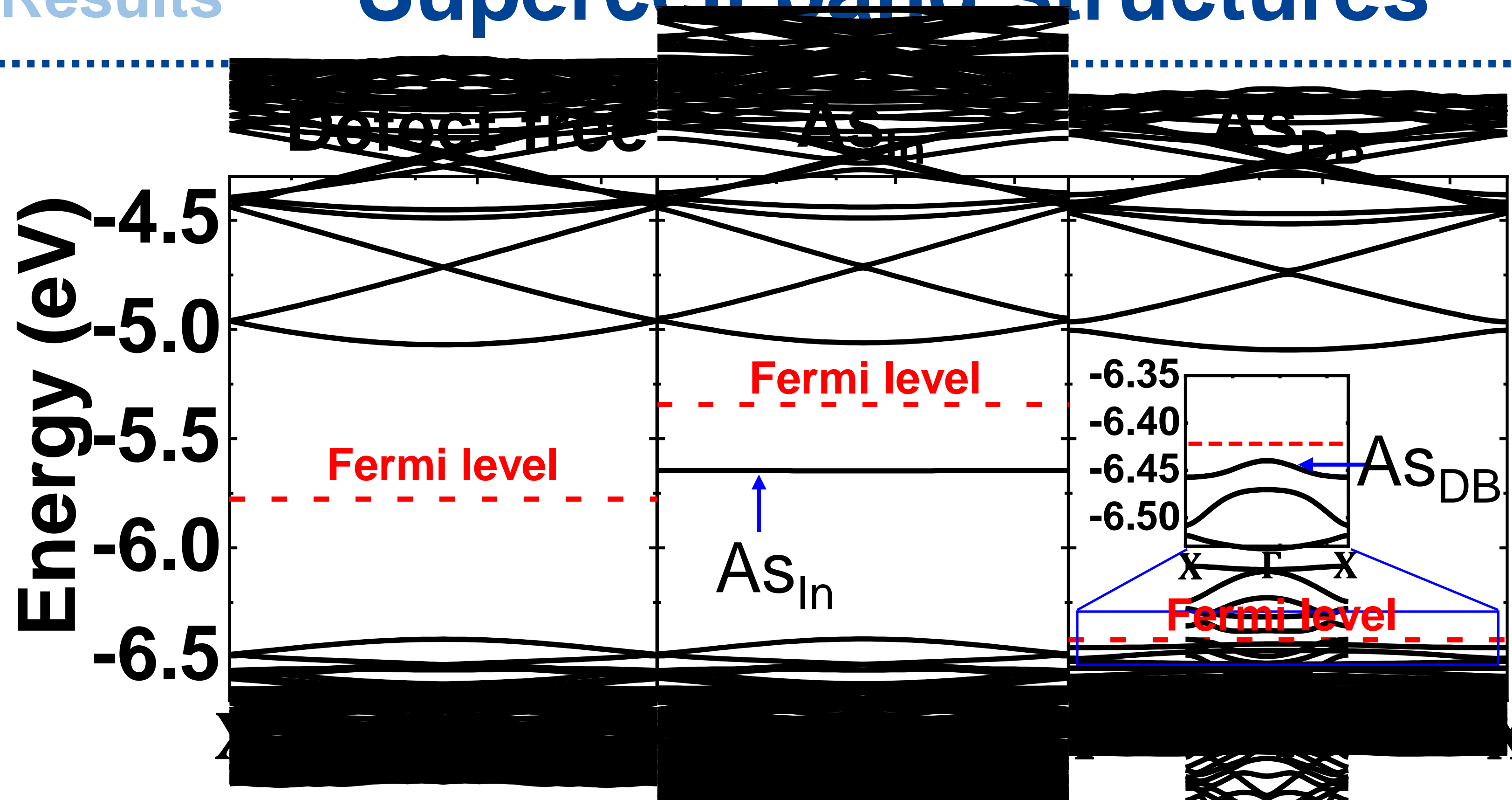
Supercell band structures



Supercell size

Defect-free : 1012 atoms

As_{In} : 1013 atoms

As_{DB} : 1012 atoms

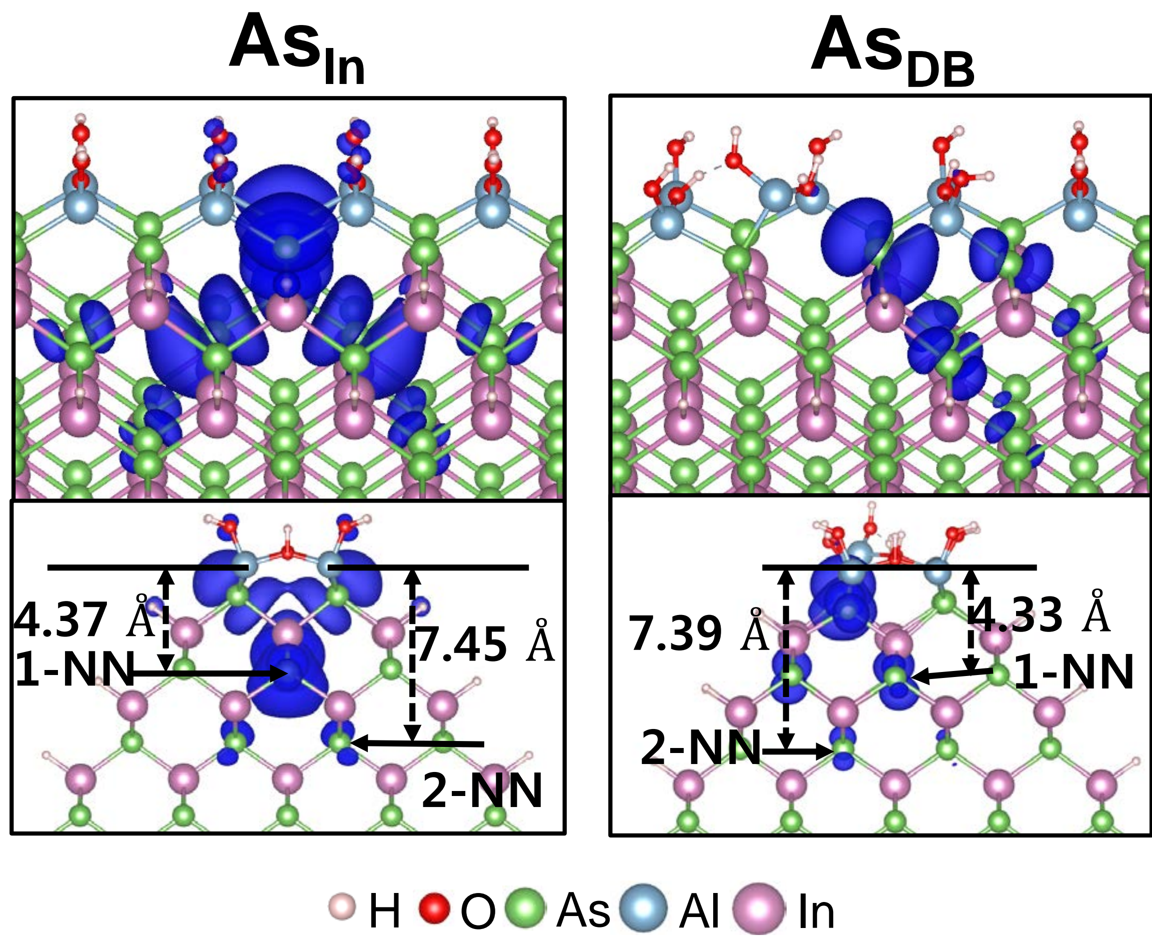
Both types of the defect are demonstrated to **be sources for the bandgap states**

→ As_{In} (**deep trap**) / As_{DB} (**shallow trap**)

Fermi level for each case is higher than the defect level

→ **Positive charges** are trapped in the defect states at nonequilibrium simulations

Local density of states of the defect states



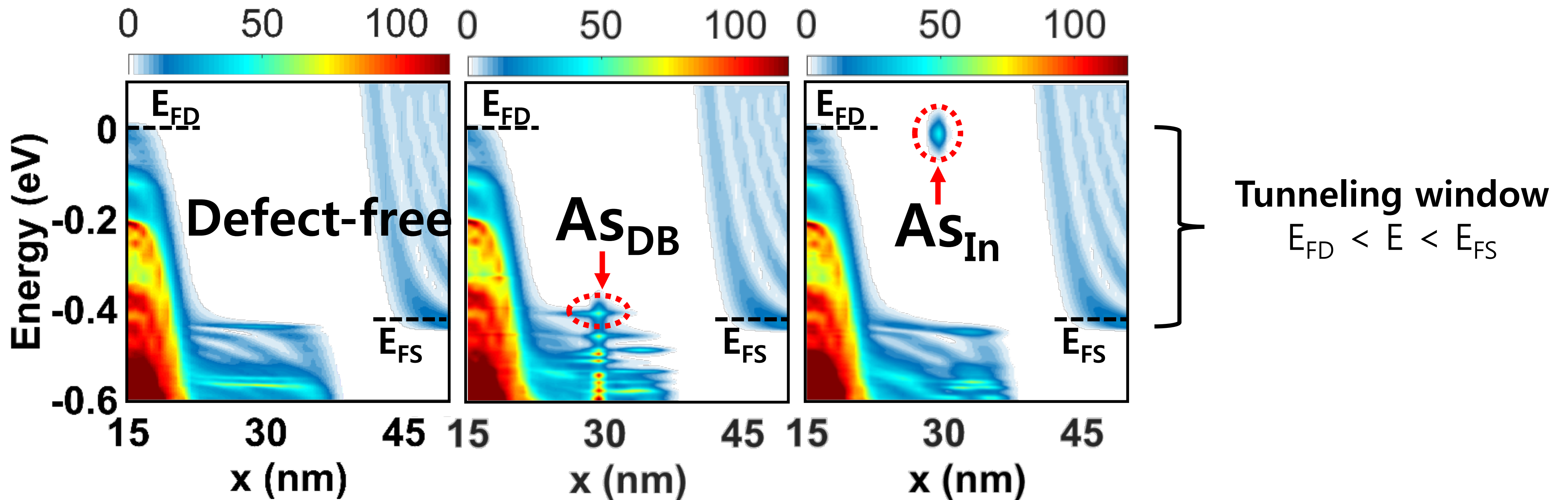
Defect LDOS largely spreads over the first nearest neighbor **(1-NN)** and the second nearest neighbor **(2-NN)** As atoms

As_{In} → 1-NN: **4 atoms**, 2-NN: **6 atoms**
As_{DB} → 1-NN: **3 atoms**, 2-NN: **3 atoms**

1-NN atoms → **4.3** Å from the interface
2-NN atoms → **7.4** Å from the interface
→ **Trapped charges in the interfacial defect permeate inside the NW**

These atomic properties of the defects can importantly affect the electrostatics of the TFET at nanoscale, influencing TFET performance

Energy-resolved DOS (NEGF)



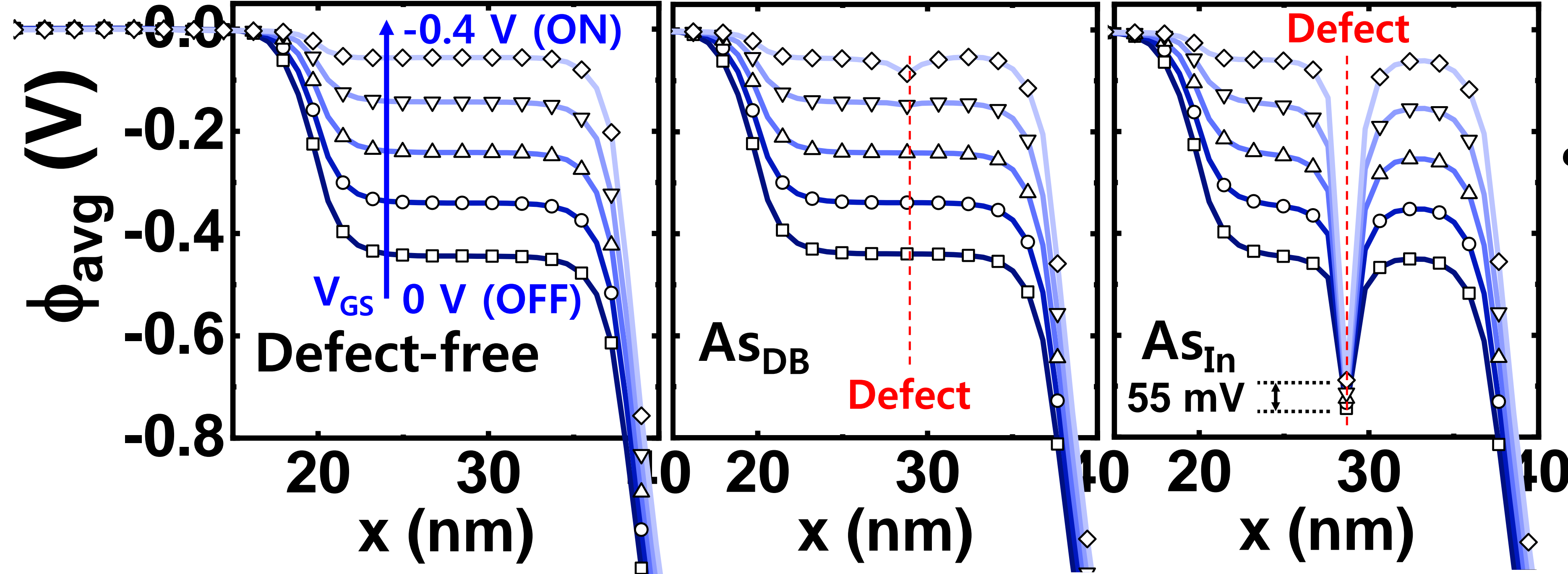
The defect states are within tunneling window → **TAT leakage current**

Deep/shallow properties agree with that of the results of DFT calculation

However, 1) **the valence band is deformed** compared with the defect-free

2) Defect level of **As_{In}** is significantly shifted down: **0.7 eV → 0.3 eV**

Density-averaged potential

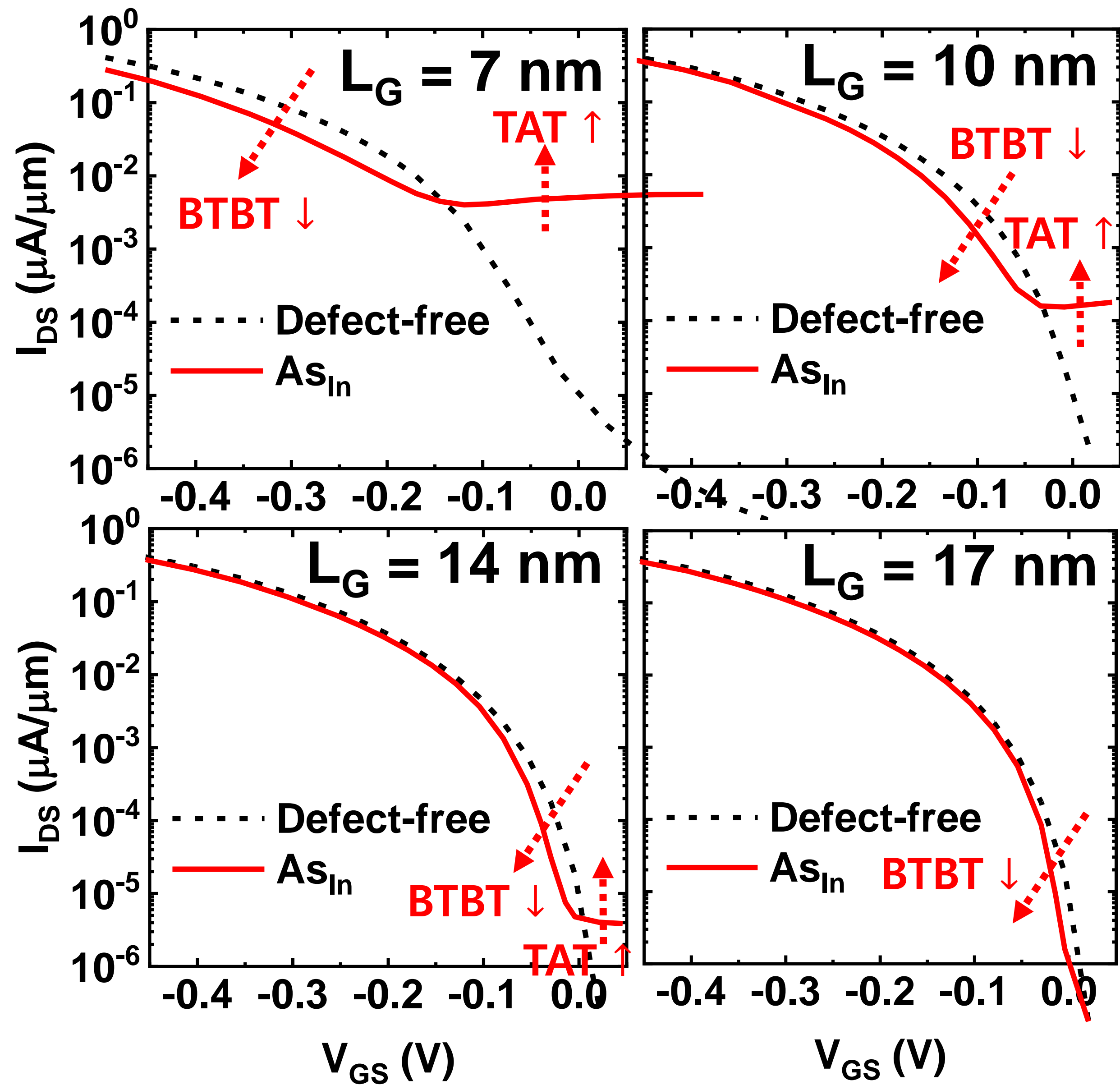


$$\phi_{avg}(x_i) = \frac{\sum_{j \in cell(i)} \phi(j) p(j)}{\sum_{j \in cell(i)} p(j)}$$

$\phi_{avg}(x_i)$: Density averaged potential
$\phi(j)$: Potential of jth atom in cell x_i
$p(j)$: Carrier density of jth atom in cell x_i

- ϕ_{avg} is **locally pulled down** near the defect cell
  → **Positive hole carriers** are trapped in the defect states
- The effect of the trapped charges is **more significant in As_{In}** than **As_{DB}**
- For As_{In}, ϕ_{avg} at the defect cell is almost unchanged
  → Trapped charges considerably **screen the gate field**

Impact of As_{In}



Impact of As_{In}

Effect 1:

Trapped charges → push down valence band edge → BTBT ↓ ➔ I_{DS} ↓

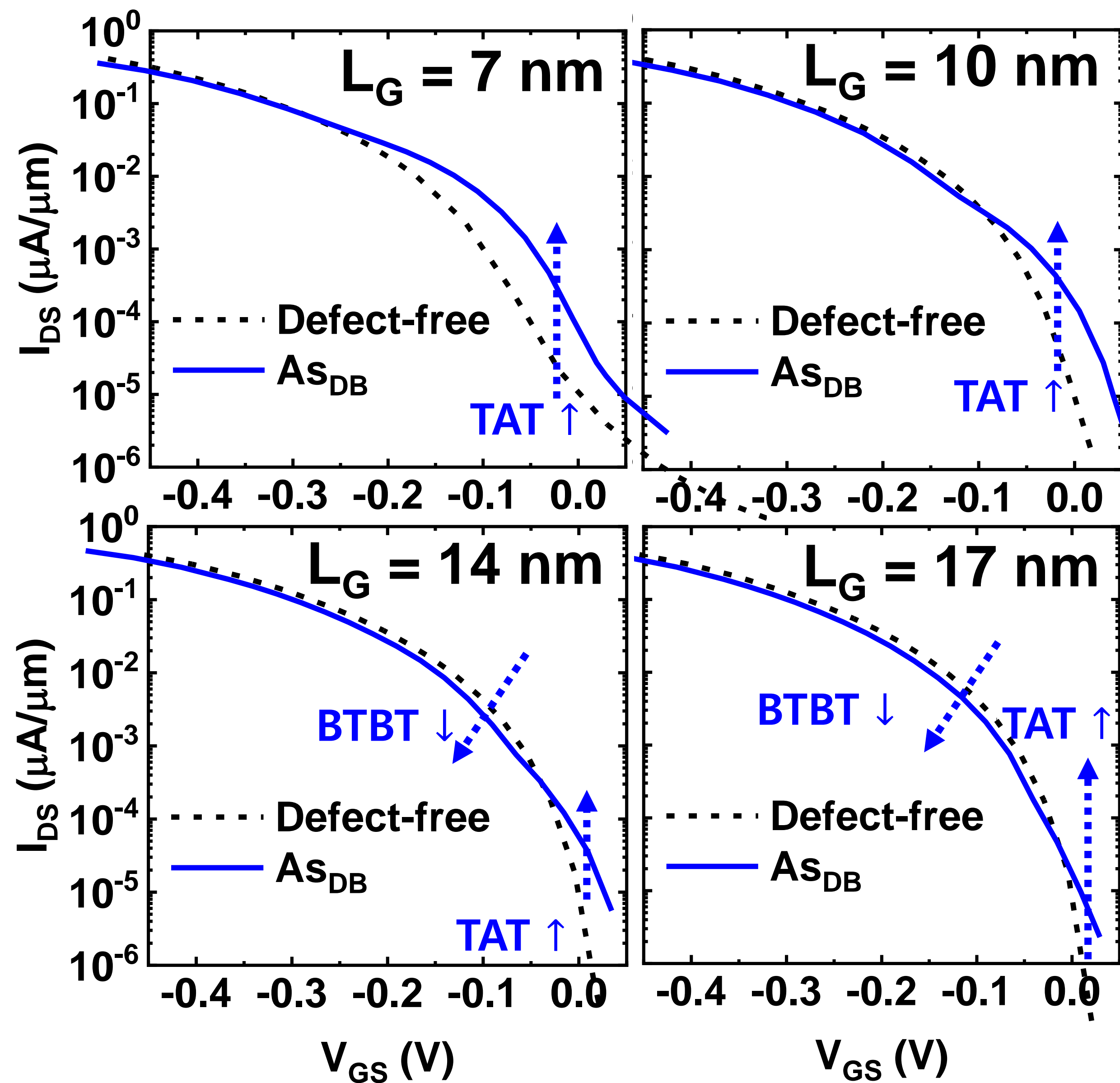
Effect 2:

Trapped charges → strong screening
→ TAT path effectively pinned at drain Fermi
➔ leakage current floor (**TAT current almost constant**)

For L_G = 17 nm, TAT is negligible due to relatively long LG → Effect 1 dominant

Effect 1, 2 becomes severe with decreasing L_G

Impact of As_{DB}



Impact of As_{DB}

Effect 1:

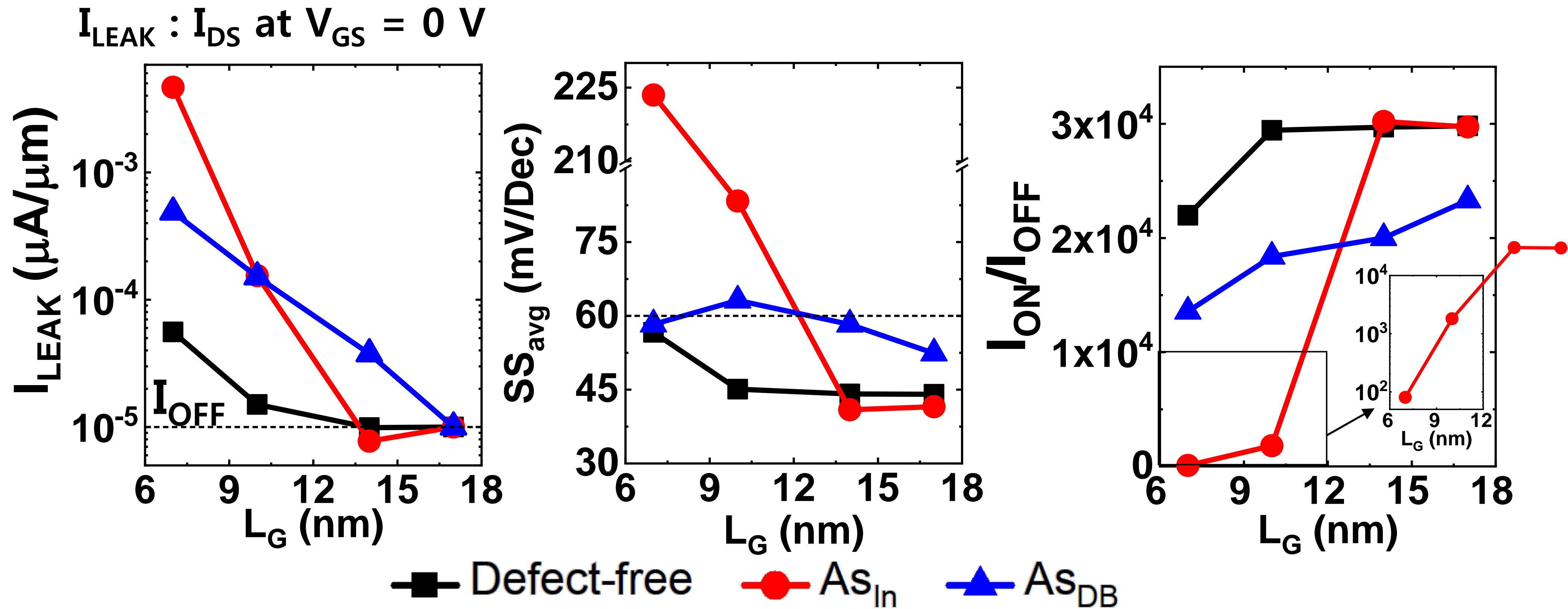
Negligible trapped charges → TAT states easily controlled by V_{GS}

➔ TAT increased with V_{GS}

Effect 2:

AsDB deforms valence band structures → BTBT ↓

Impact of a defect on L_G scaling



The detrimental defect depends on L_G scaling range

- Deep L_G scaling (L_G < 12 nm) : **As_{DB}**
- Moderate L_G scaling (L_G > 12 nm) : **As_{In}**

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Conclusions

- We investigated the impacts of single interfacial defects that creates bandgap states, As_{In} and As_{DB}, on InAs GAA NW TFET at nanoscale
- The atomic properties of individual defects are rigorously investigated employing the DFT defect Hamiltonians
  → Charge trapping at interfacial defects can permeate inside the NW, not negligible for the nanoscale device
- Critical defect limiting scaling depends on L_G range