nanoHUB online simulation and more

an NCN project

Network for Computational Nanotechnology (NCN)

Berkeley, Univ.of Illinois, Norfolk State, Northwestern, Purdue, UTEP

Performance Limitations of Graphene Nanoribbon Tunneling FETS due to Line Edge Roughness

Mathieu Luisier and Gerhard Klimeck

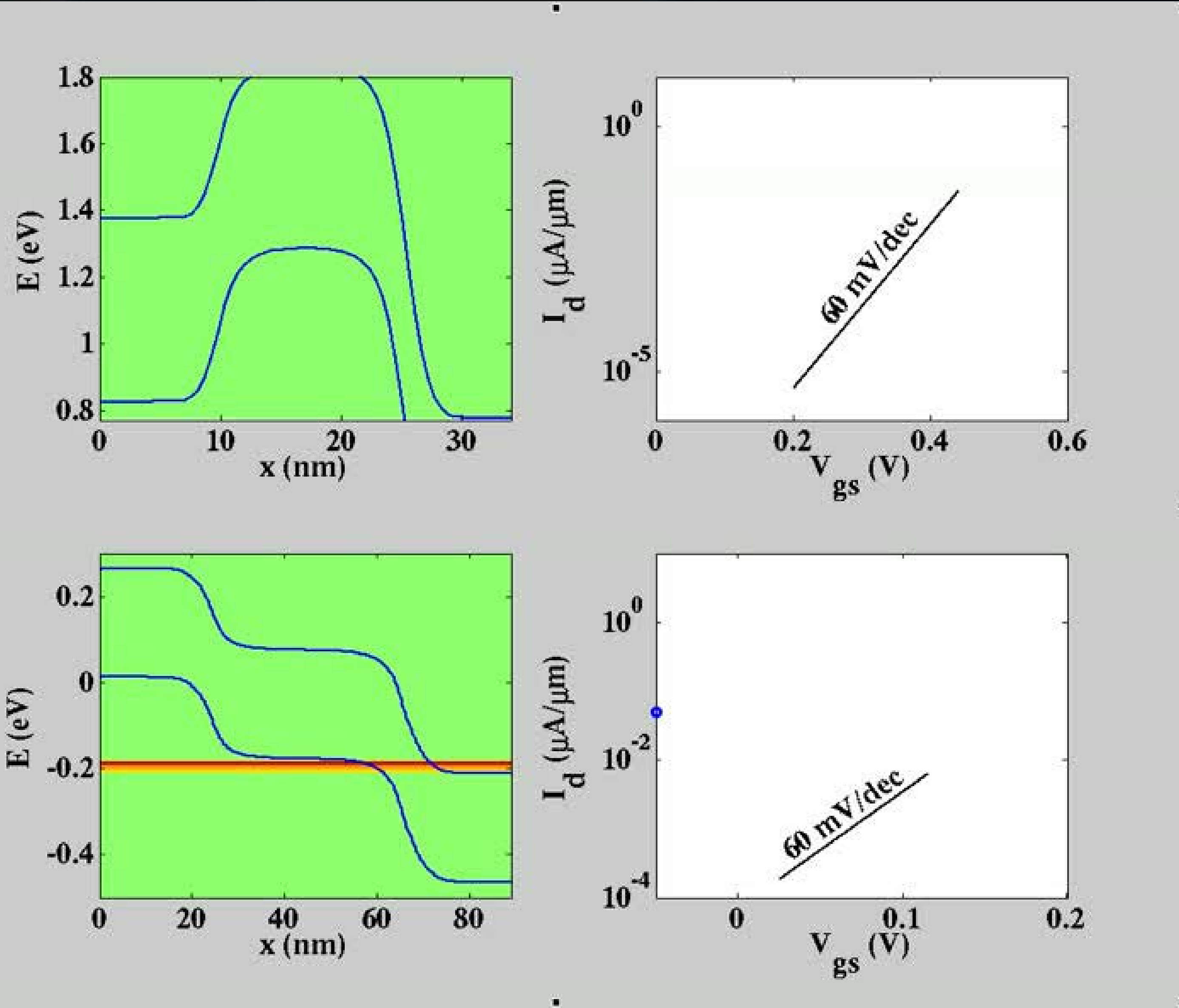
NCN

PURDUE UNIVERSITY

NCN NSF

Motivation

Tunneling Transistor after MOSFET?



MOSFET: Thermionic Current

TFET: B-to-B Tunn. Current

Graphene Nanoribbon TFETs

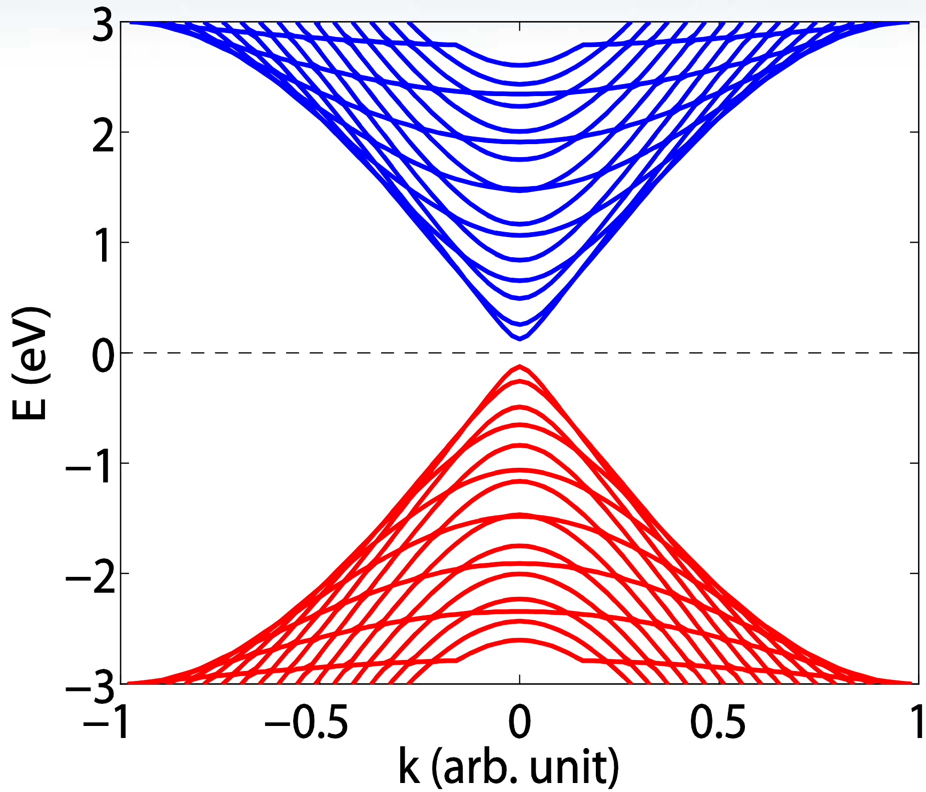
Graphene Nanoribbon:

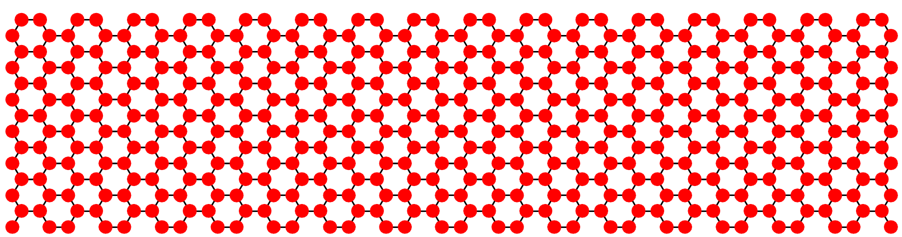
GOOD:

- One-Dimensional Structure
- Compatible to Planar Tech.
- Low Effective Masses
- Tunable Band Gap (Width)

BAD:

- Band Gap => Narrow Ribbon
- Edges => Roughness





Bandstructure of 5.1nm GNR
Symmetric CB and VB
Band Gap E_g = 0.251 eV

Overview

- Introduction
- Physical Models
    - Bandstructure and Transport Models
- Ideal Graphene Nanoribbon
    - Structure Definition and Optimization
    - Transfer Characteristics
- Line Edge Roughness
    - Roughness Generation
    - Band Gap Reduction
    - Performance Deterioration
- Conclusion and Outlook

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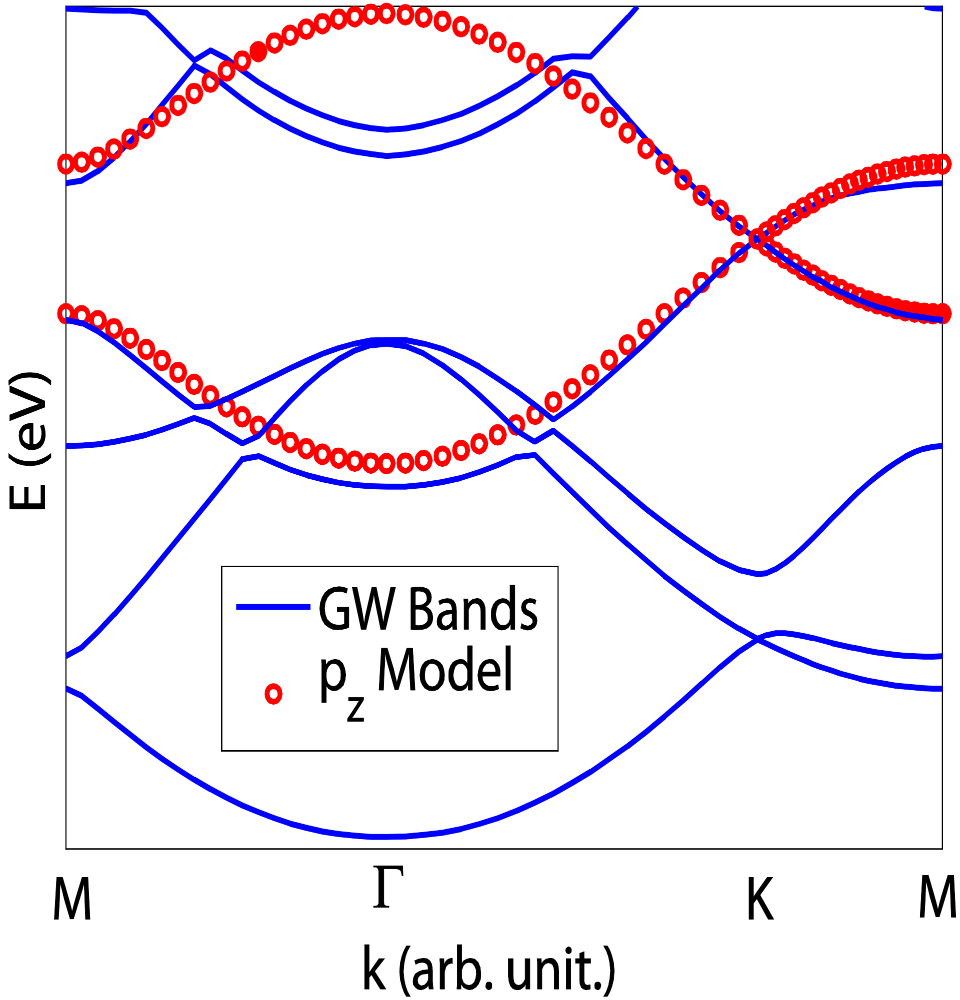
Nearest-Neighbor p_z Tight-Binding Method

GOOD:

- one single parameter $V_{pp\pi}$
- HOMO and LUMO bands
- *atomistic* description
- computationally efficient

BAD:

- not really full-band



Quasi 3D Schrödinger Equation

$$\mathbf{H} \,|\, \psi_E > \;=\; E \,|\, \psi_E >$$

Tight-Binding Ansatz for the Wave Function

$$< \mathbf{r} \,|\, \psi_E > \;=\; \sum_{ijk} C_{ijk}(E)\Phi(\mathbf{r} - \mathbf{R}_{ijk})$$

$$(E\text{-}H\text{-}\Sigma)\cdot G^R = I$$

Matrix Inversion Problem

$$(E\text{-}H\text{-}\Sigma)\cdot C = Inj$$

Linear System of Eq.

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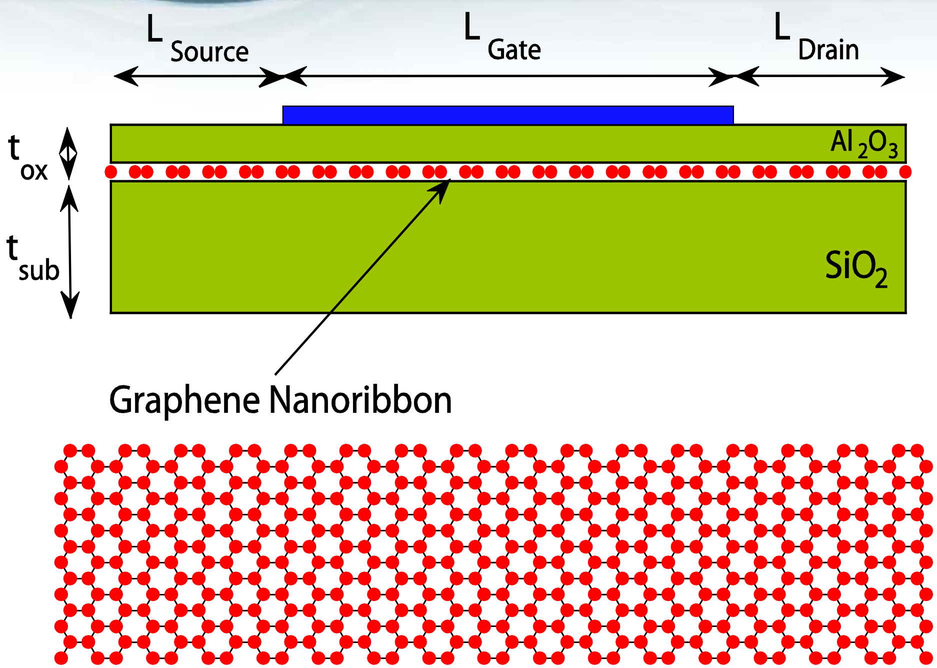
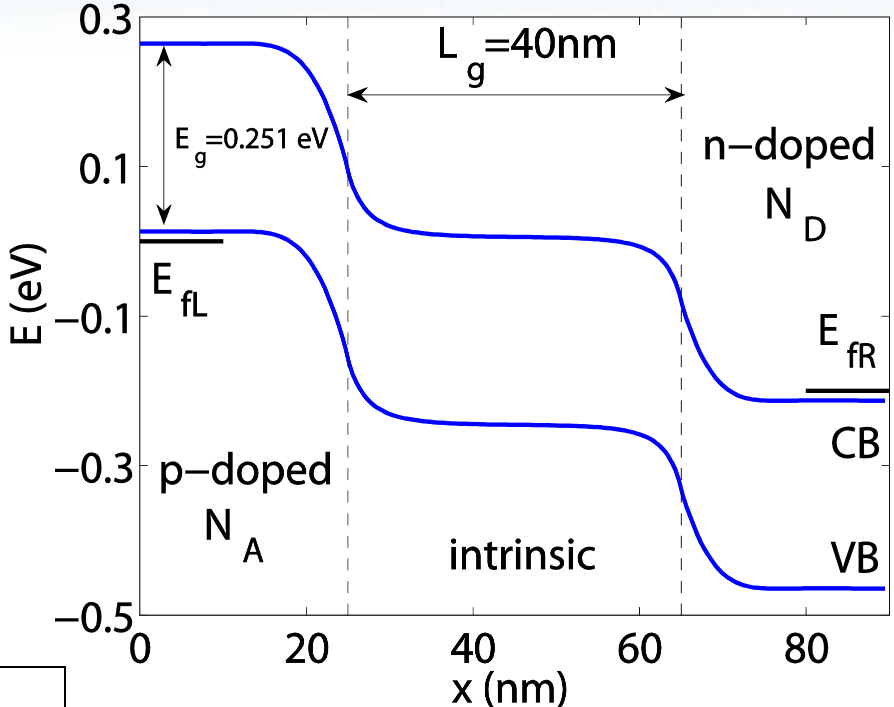
Ideal Structure (1)

Graphene Nanoribbon with Armchair Edges





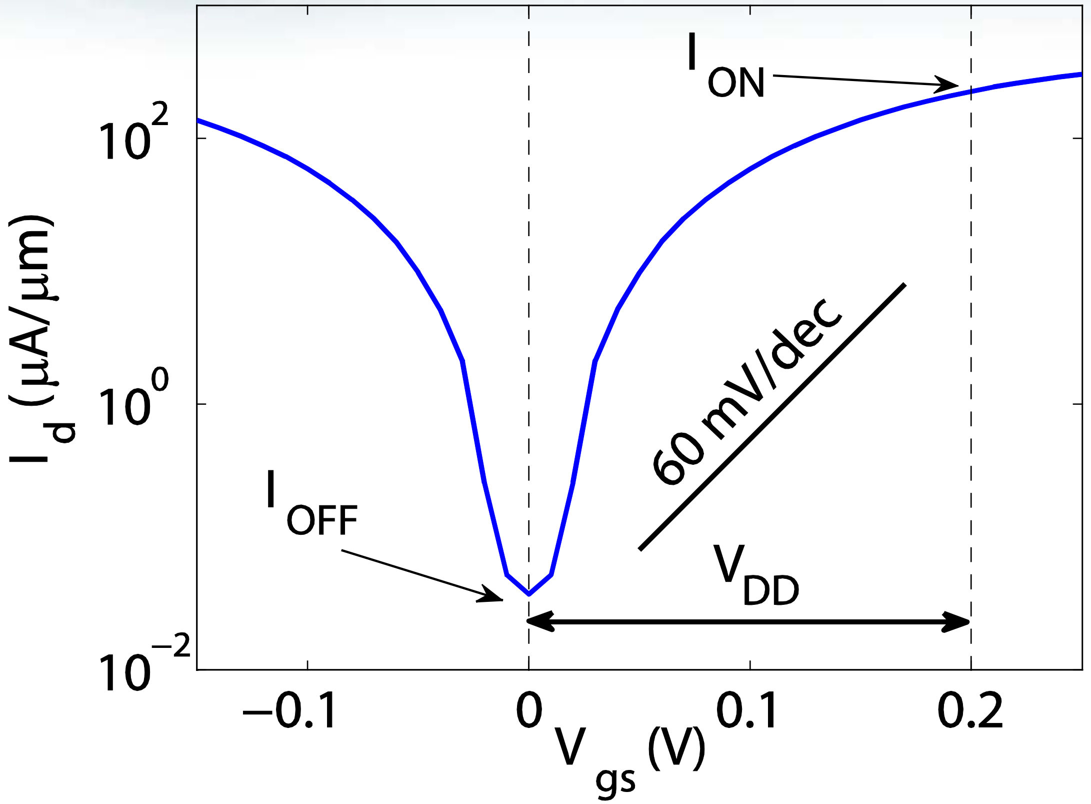
TFET p-i-n Structure:

- 5.1nm GNR Deposed on SiO_2 (N=21)
- 1nm EOT (2.35nm Al_2O_3 with ε_R=9.1)
- 40nm Gate Length
- 25nm Source and Drain Extensions

- Supply Voltage V_{DD}=0.2 V
- Symmetric Doping Conc.
- GNR Band Gap E_g=0.251 eV

Ideal Structure (2)

I_d-V_{gs} Transfer Characteristics



ON-Current:
I_{ON}=225 μA/μm

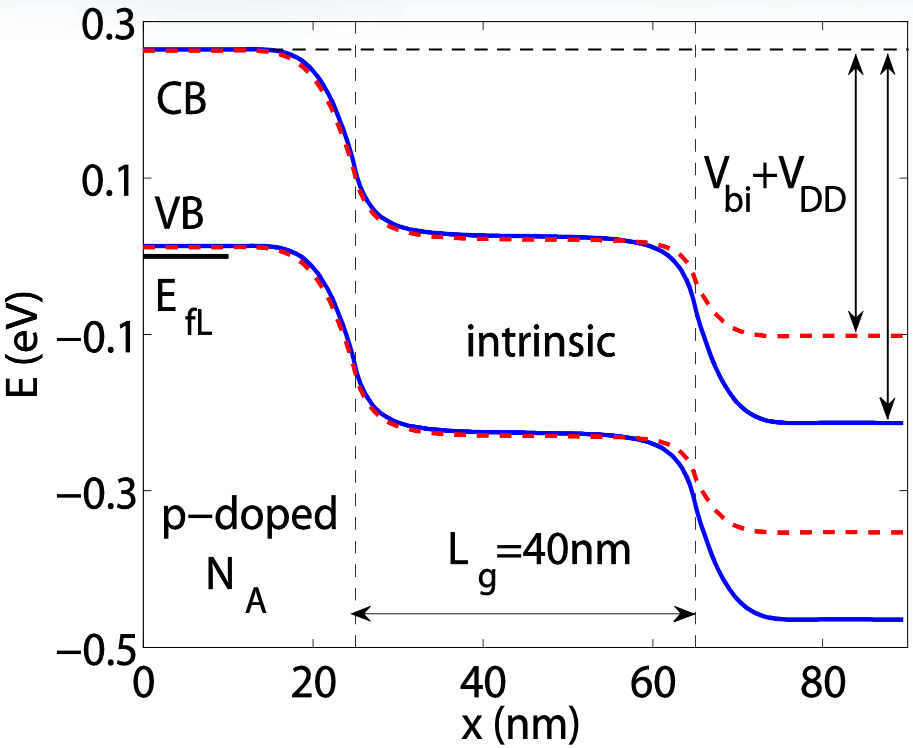
OFF-Current:
I_{OFF}=37 nA/μm

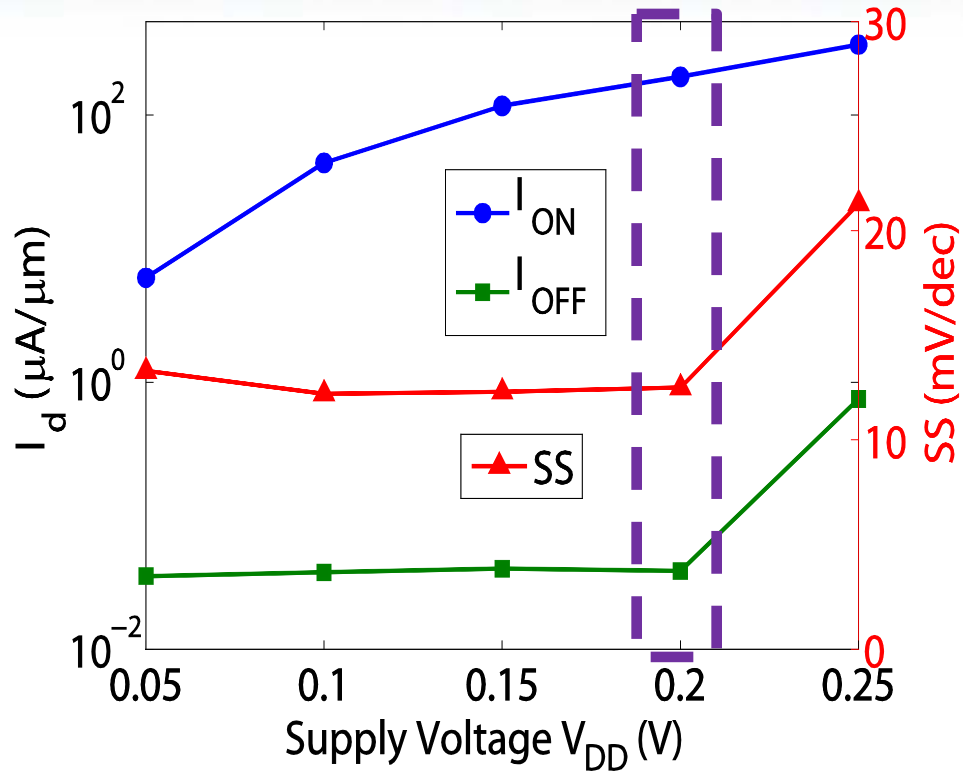
Subthreshold Slope
SS=12 mV/dec

1) How can we decrease the OFF-Current?
2) How can we increase the ON-Current?

Ideal Structure (5)

Determination of Supply Voltage





- **ON-Current Increases with V_{DD} (due to Gate Voltage)**
- **Condition $V_{bi}+V_{DD}<2*E_g$ must be Satisfied**
- **Condition Broken => Ambipolar Channel Behavior**

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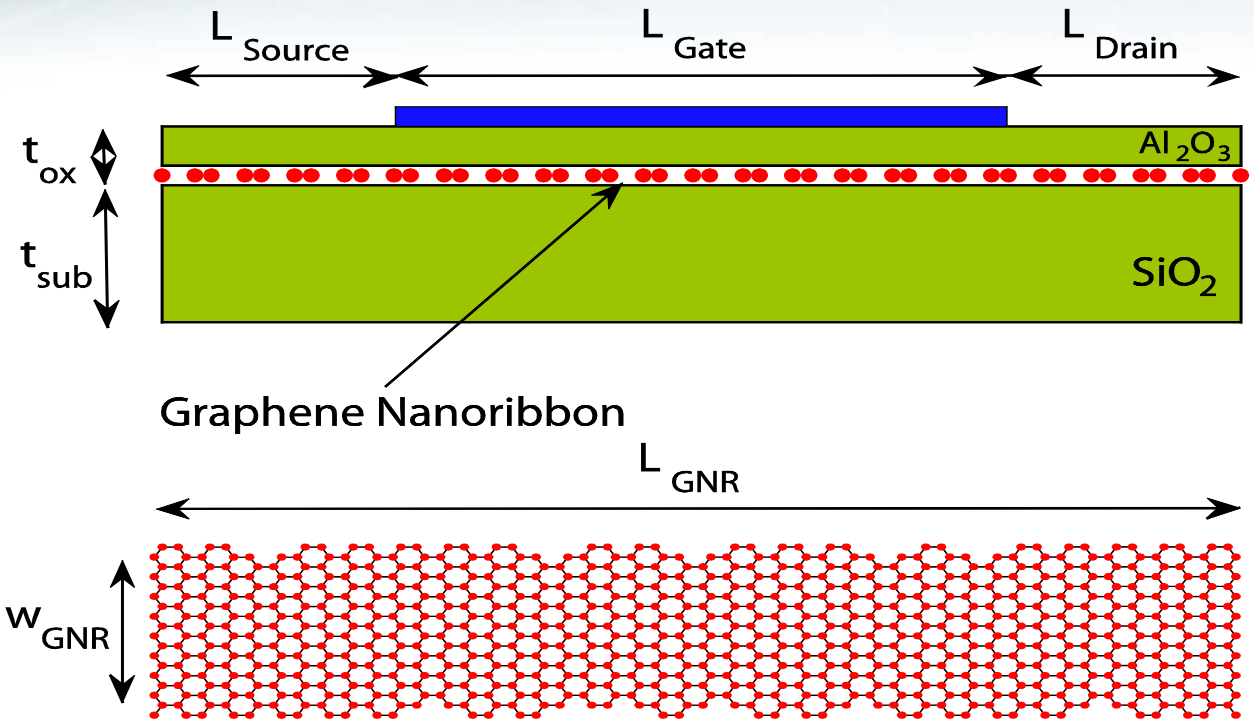
Rough Structure (1)

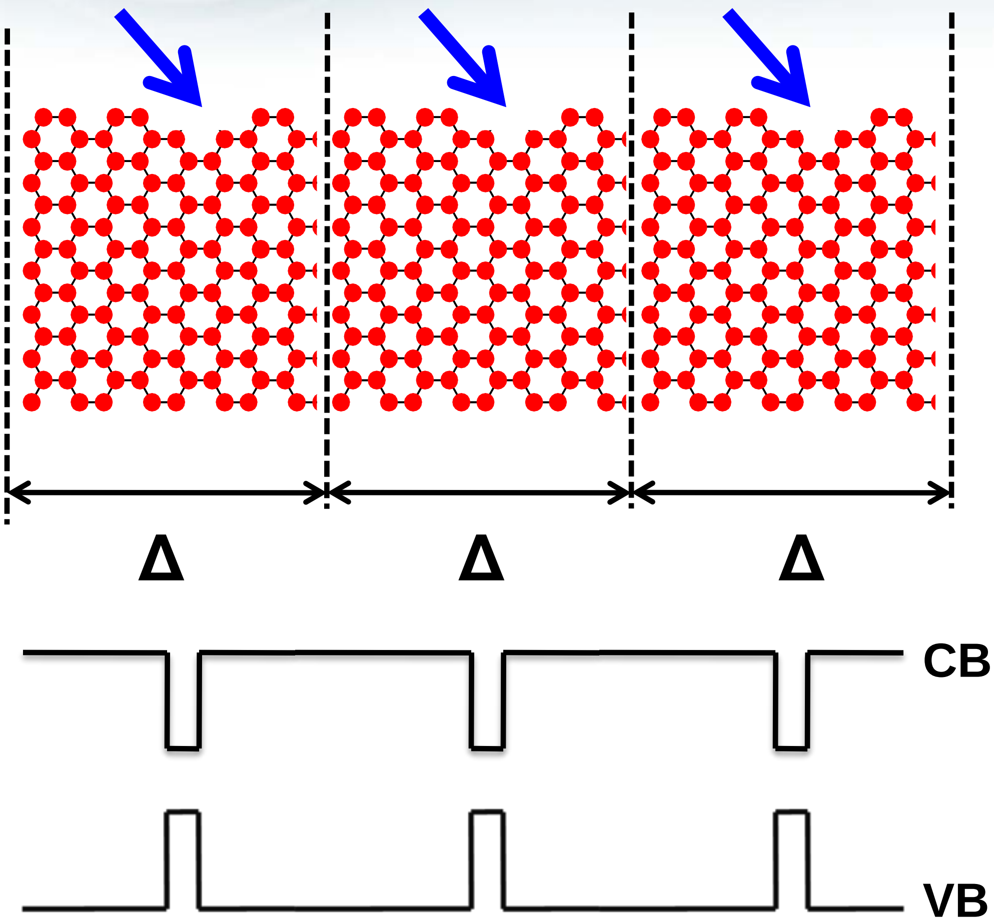
Structure Definition

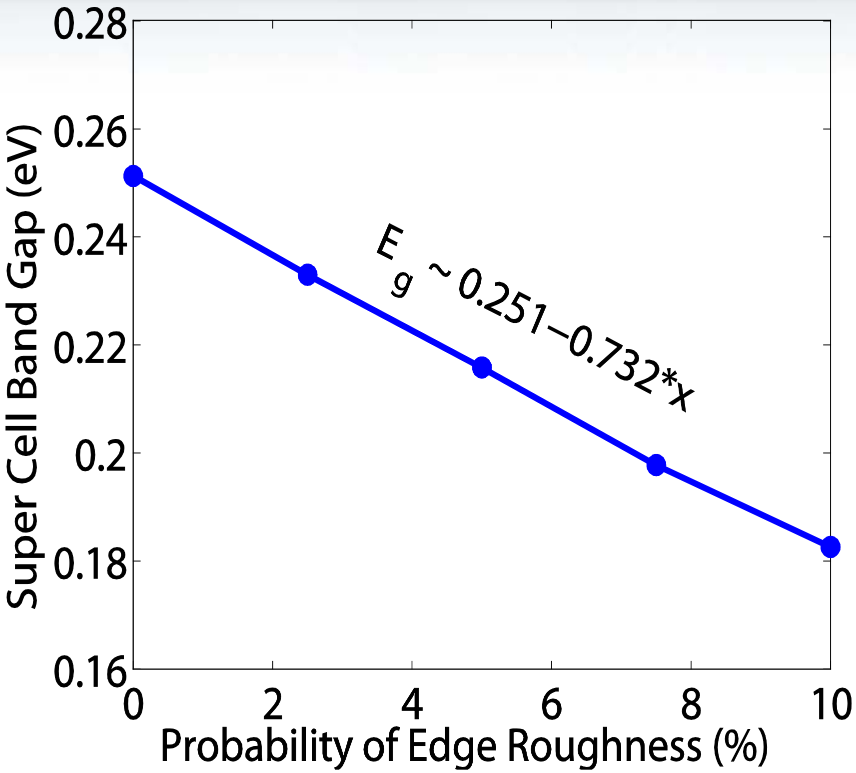


- **No Perfect Edges => Line Edge Roughness (LER) Scattering**
- **Simple Roughness Model: Remove Pair of Atoms with Probability P**
- **Random Distribution of Removed Atoms: N=21 to N=20**

Rough Structure (2)

Band Gap Reduction



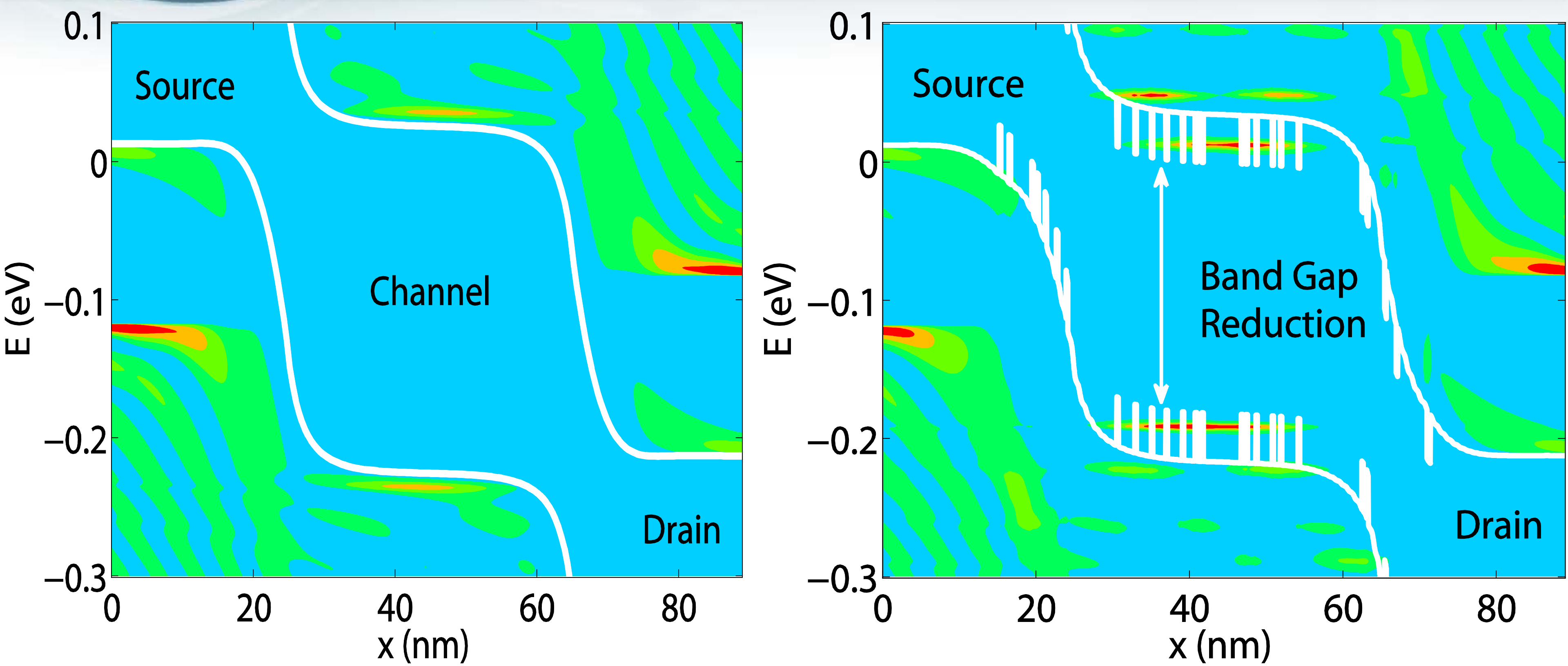


Edge Defect => Symmetry Broken
Band Gap Reduction
~Linear Dependence on P

Periodic Structure with 1 Defect/Period

Rough Structure (3)

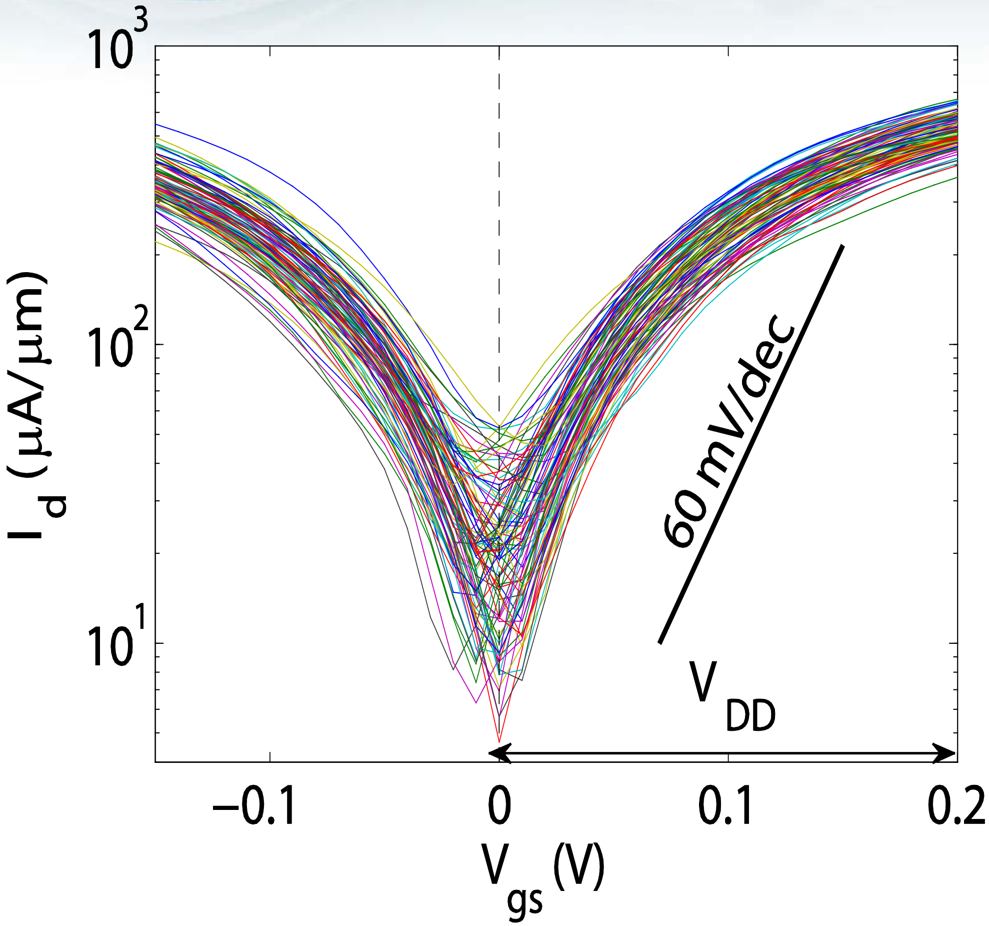
GNR Density-of-States



- **Spectral Density-of-States Around the Intrinsic Channel w and w/o LER**
- **Band Gape Reduction => Superlattice Structure => BG Localized States**
- **Localized States => Increased B-to-B Tunneling Probabilities**

Rough Structure (4)

Multiple Random Samples Generation

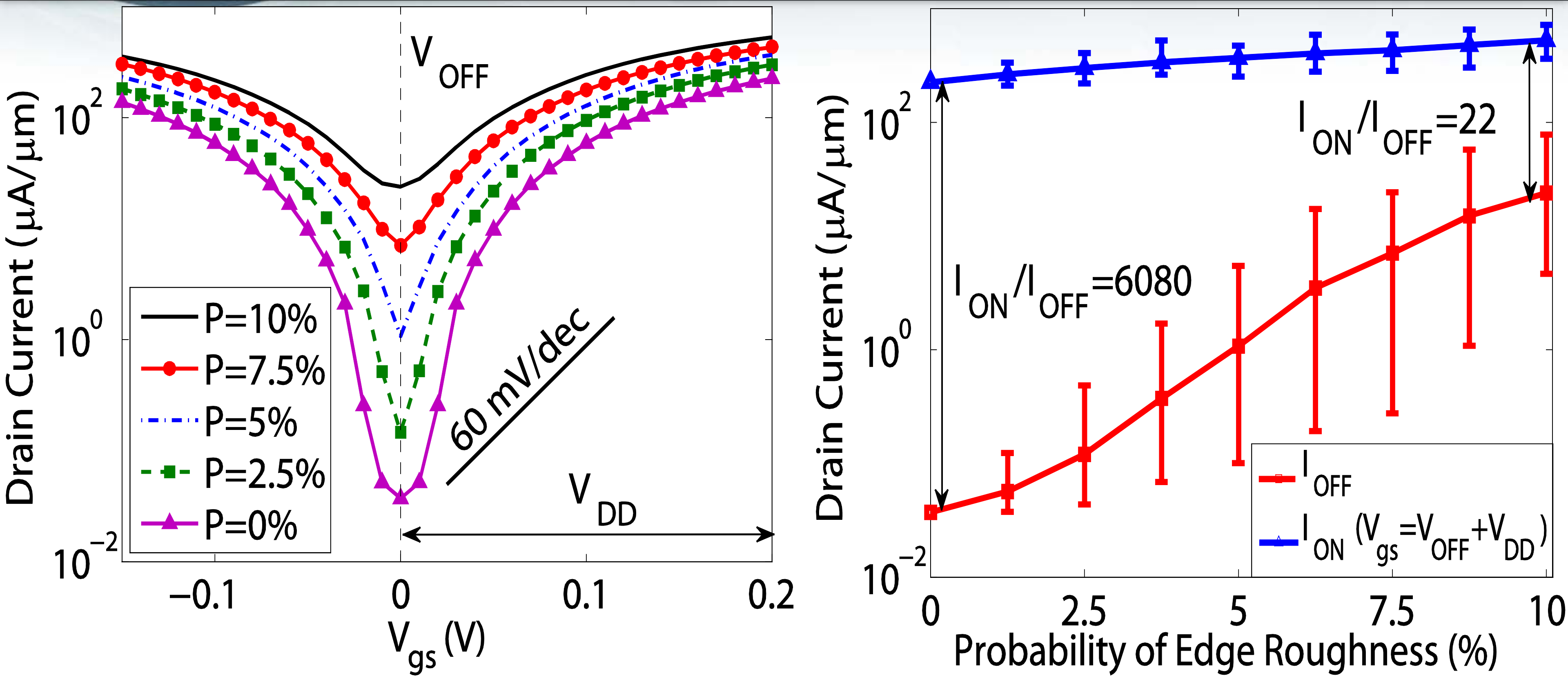


- **Roughness Probability P from 0 to 10%**
- **Statistical Sampling of LER (100 Samples per Roughness Probability)**
- **All Devices Different**
- **Need: Average ON- and OFF-Currents, Standard Deviations, and Max and Min Values**

Graphene Nanoribbon TFETs with 10% of Edge Atoms Removed => Strong Variation of ON- and OFF-Currents, Poor Performances

Rough Structure (5)

Transfer Characteristics and I_{ON}/I_{OFF} Ratio



- **Comparison of GNR TFETs with Different LER Probabilities**
- **Strong Deterioration of Most Device Performances**
- **Better Control of Edges or Better Structure Optimization**

Conclusion and Outlook

- **GNR TFET Simulation**
  - **p_z Tight-Binding Orbital Model**
  - **3D Schrödinger-Poisson Solver**
- **Device Simulation**
  - **Structure Optimization (Doping, L_g, V_{DD})**
  - **LER => Localized Band Gap States**
  - **LER => Performance Deterioration**
- **Outlook and Challenges**
  - **Ripples Scattering**
  - **More Accurate Bandstructure Model**
  - **Dissipative Scattering (El-Ph)**