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Treatment of Point Defects in Nanowire MOSFETs Using the Nonequilibrium Green's Function Formalism

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Outline

- Introduction
  - MOSFETs downscaling: statistical fluctuations of doping impurity positions
- 3D Quantum simulation of point defects in nanowire transistors
  - Nonequilibrium Green Function formalism: Mode-Space approach
  - Treatment of point defects
- Results: influence of the impurity location and type
  - Energy subbands
  - Transverse modes
  - Current characteristics
- Conclusions and perspectives

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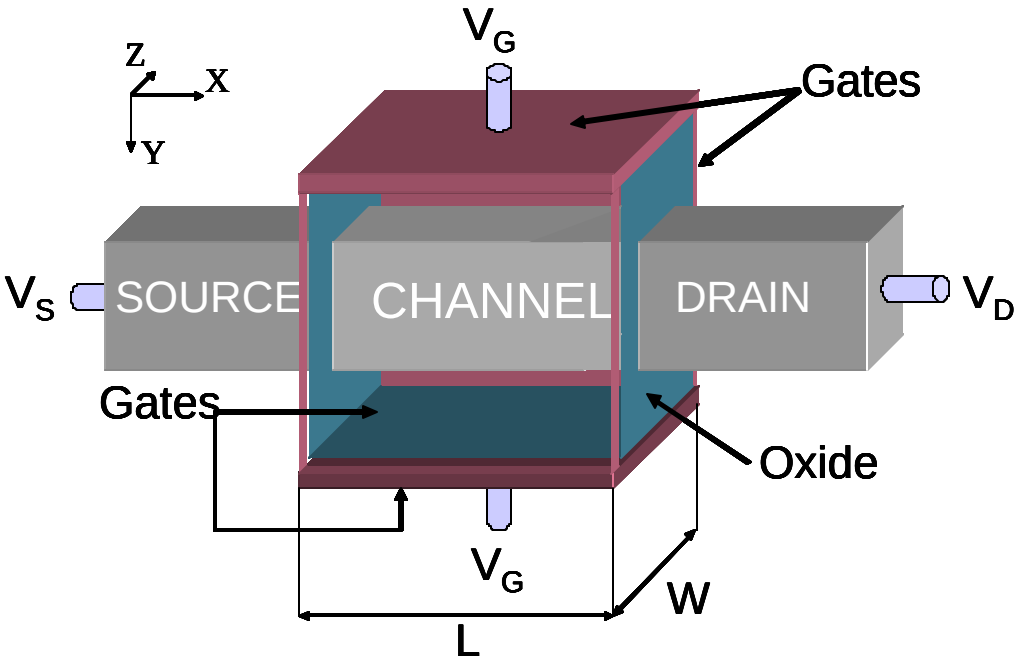
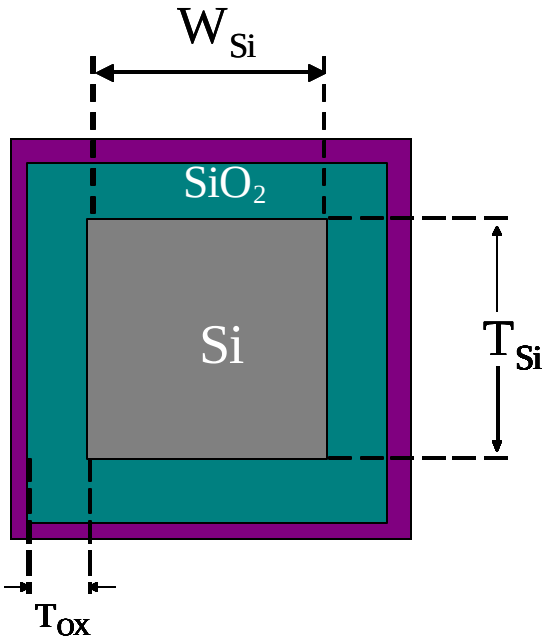
Dimensions of nanowire MOSFETs





- ✓ Source and drain region: continuous doping of 10^{20} cm^{-3}.
- ✓ Dimensions: L=8 nm, W_{Si}=3 nm, and T_{Si}=3 nm, T_{OX}=1 nm.
- ✓ Channel region: discrete doping of 10^{19} cm^{-3}, with 1 impurity on average.

Þ **Effect of the impurity type and location.**

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Nonequilibrium Green's function formalism

Point Defect Treatment

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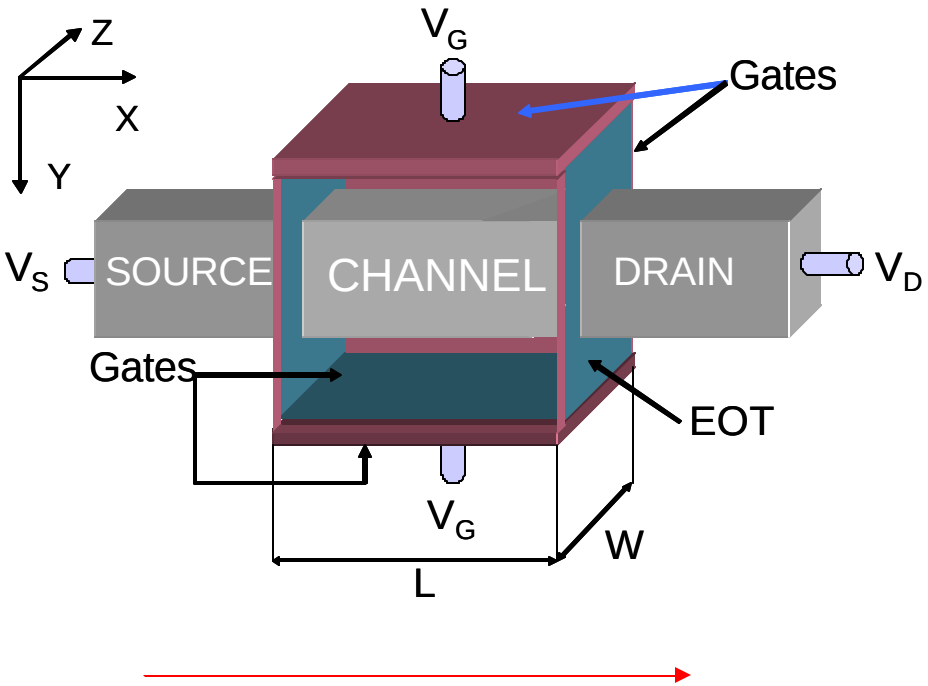
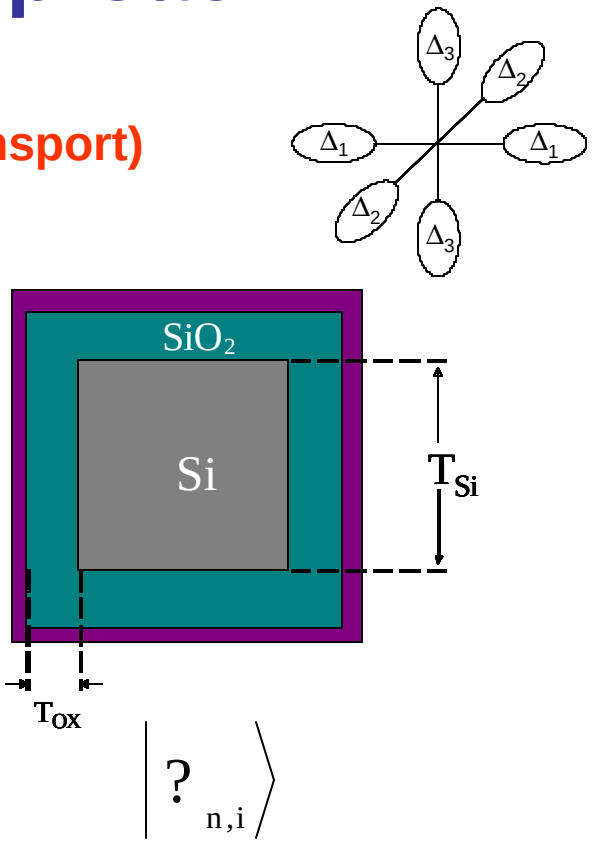
The 3D Mode Space Approach*

- The 3D Schrödinger = **2D (confinement)** + **1D (transport)**





i^{th} eigenstate of the n^{th} atomic plan

- **Hypothesis: $y_{n,i}$ is constant along the transport axis.**

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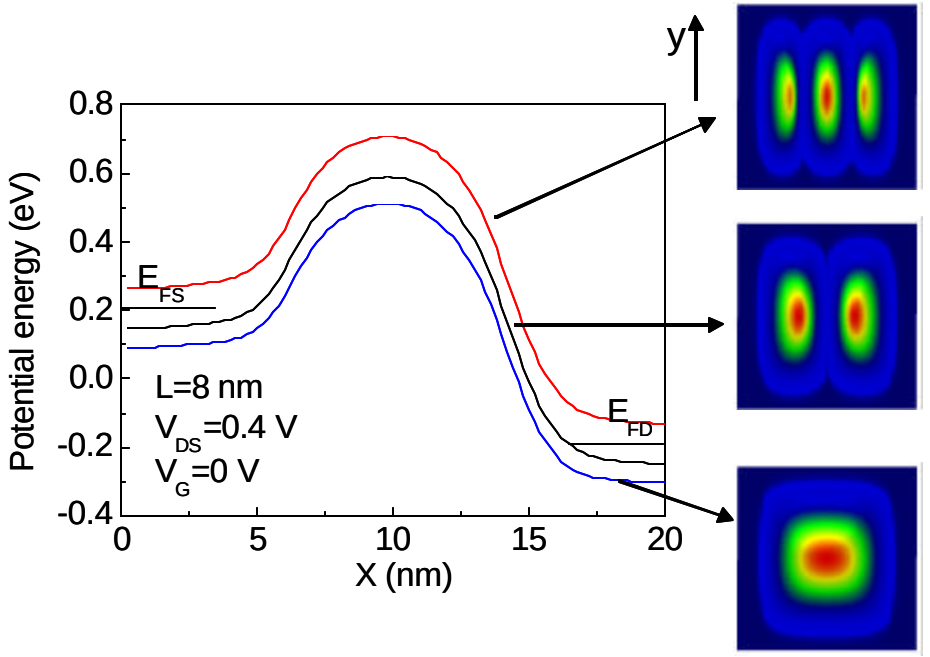
* J. Wang *et al*. J. Appl. Phys. **96**, 2192 (2004).

The 3D Mode Space Approach

- Electron distribution along subbands (valley (010)):



- For each subband i:

$\left| ?_{n,i} \right\rangle$: Transverse eigenstate

$e_{n,i}$: Transverse eigenvalue

$G_i(e)$: 1D Green function

- Simplified tight-binding approach: cubic lattice with a_x, a_y, a_z.

  - 1 orbital/atom: $\left| l, m, n \right\rangle$: position $z=l\times a_z$, $y=m\times a_y$, $x=n\times a_x$.
  - Interactions between first neighbors.

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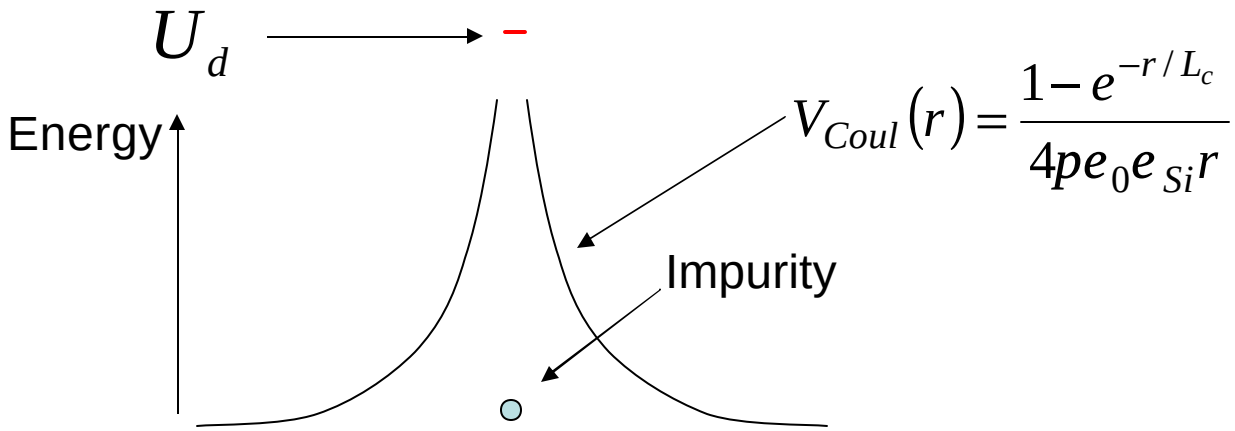
Point defect description



- Point Defect = On-site Potential + Coulomb Tail

Treated as a localized variation
= Chemical structure

⇒ Included in the real space approach based on the Dyson equation.
[$G=(I-G_0V)^{-1}G_0$]

Treated as a macroscopic variation

⇒ Included in the self-consistent mode-space approach without coupling the electron subbands

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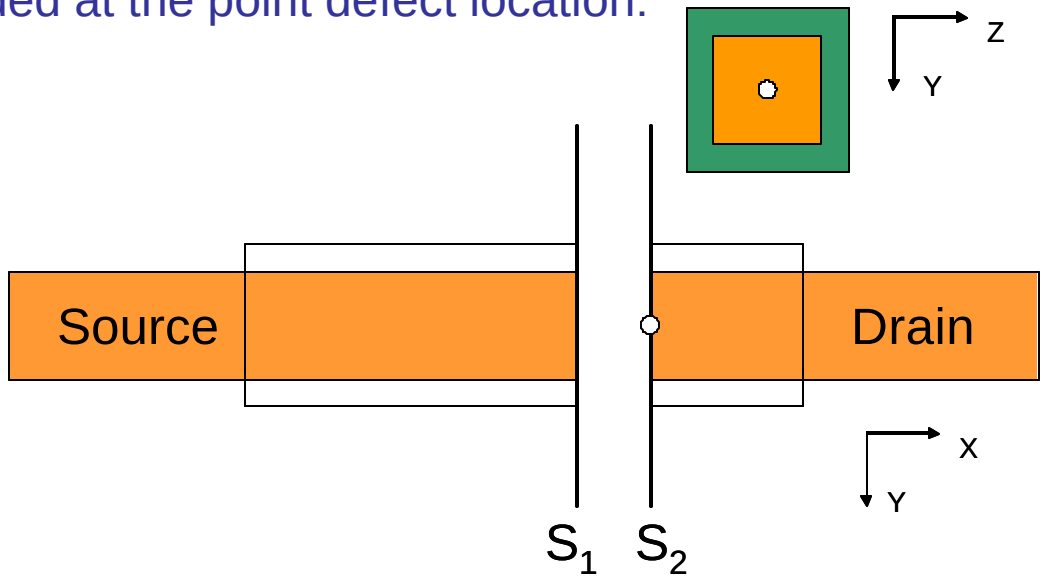
Treatment of on-site potential

- After achieving self-consistence including the Coulomb Tail, the device is subdivided at the point defect location:



- Calculation of the Green's functions of the surfaces S_1 and S_2:

$$\left\langle l_1, m_1, n_1 \left| G_{S1}(e) \right| l_1', m_1', n_1' \right\rangle = \sum_i ? \left\langle l_1, m_1, n_1 \left| ?_{n_1,i} \right\rangle \left\langle ?_{n_1,i} \left| G_i^1(e) \right| ?_{n_1',i} \right\rangle \left\langle ?_{n_1',i} \right| l_1', m_1', n_1' \right\rangle$$

$$\left\langle l_2, m_2, n_2 \left| G_{S2}(e) \right| l_2', m_2', n_2' \right\rangle = \sum_i ? \left\langle l_2, m_2, n_2 \left| ?_{n_2,i} \right\rangle \left\langle ?_{n_2,i} \left| G_i^2(e) \right| ?_{n_2',i} \right\rangle \left\langle ?_{n_2',i} \right| l_2', m_2', n_2' \right\rangle$$

Treatment of on-site potential

- U_d is then included using the Dyson equation:

$$G'_{S2}(e) = \left(I - G_{S2}(e)U\right)^{-1} G_{S2}(e)$$

Intra-atomic potential matrix

- Retarded Green function of the uncoupled system:

$$G_S^0(e) = \begin{bmatrix} G_{S1}(e) & 0 \\ 0 & G'_{S2}(e) \end{bmatrix}$$

- Calculation of the current*:

$$I = -\frac{4pe}{\hbar}\int_{-\infty}^{+\infty} de\, Tr_1\left[N_{11}^0 \Lambda_{11}^+ V_{12} N_{22}^0 V_{21} \Lambda_{11}\right]\left(f_S(e) - f_D(e)\right)$$

$$N^0 = \left[-\frac{1}{p}\mathrm{Im}\left(G_S^0\right)\right] \qquad V = \begin{bmatrix} 0 & H_{12} \\ H_{21} & 0 \end{bmatrix} \qquad \Lambda = \left[I - G_S^0 V G_S^0 V\right]^{-1}$$

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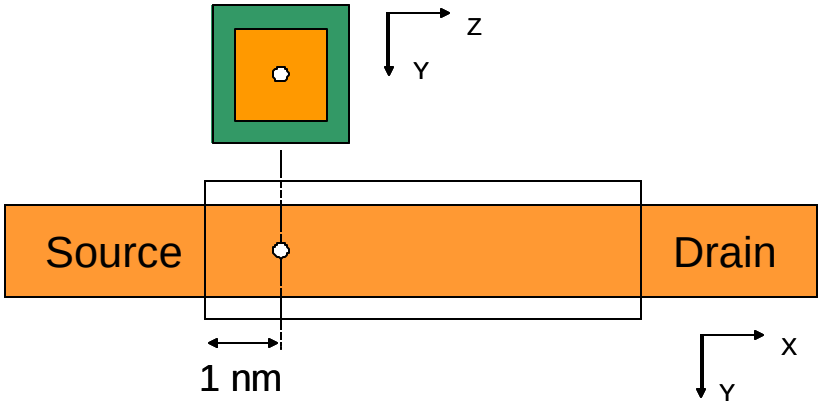
* M. Bescond *et al.*, Solid-State Electron. **48**, 567 (2004).

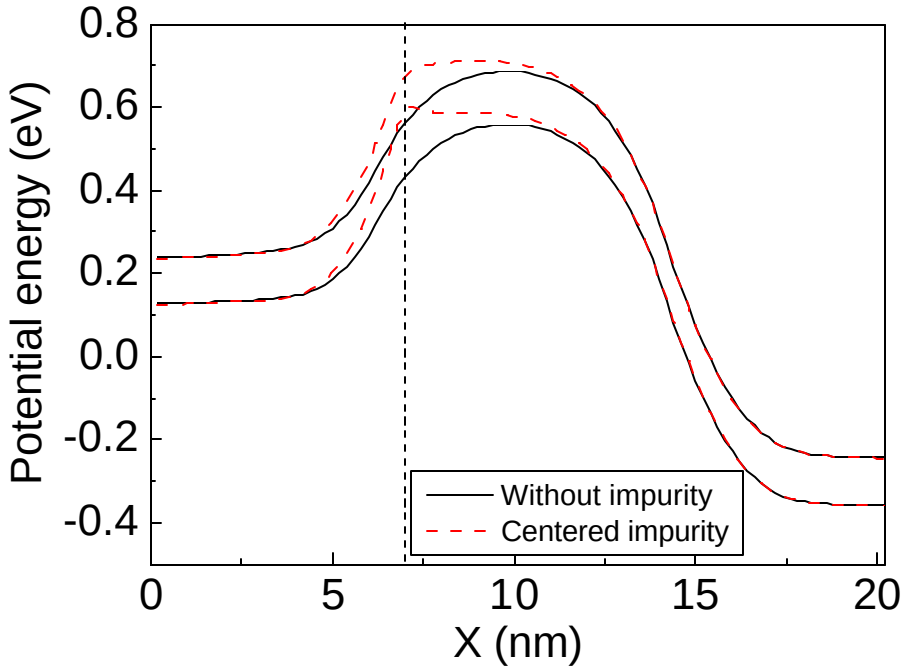
Results

Influence of point defect

Simulation results

- Electronic subbands: Effect of the Coulombic potential (valley (010))





✓ Subband profile is affected by the impurity.
✓ Subbands are still independant: justification of the mode-space approach.
✓Acceptor impurity increases the channel barrier.

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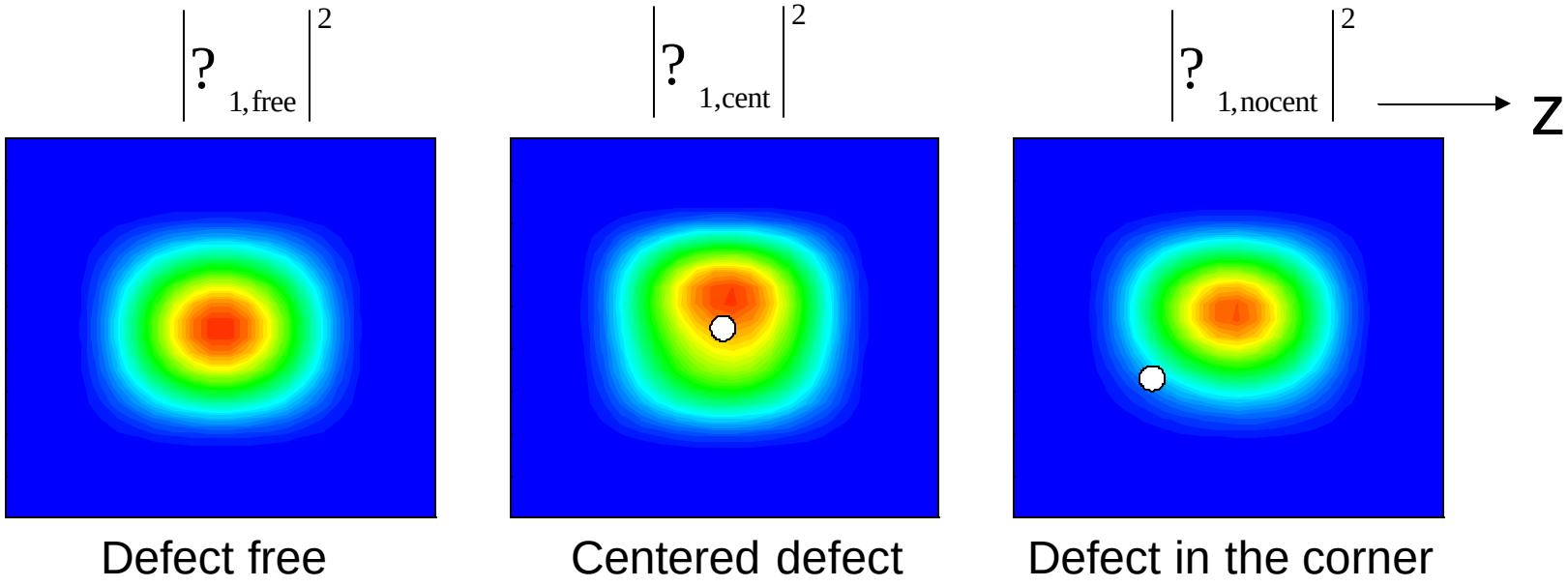
Simulation results

- Evolution the 1st confinement eigenstate (valley (010)):



- ✓ Highest variations of the eigenstate with centered impurity.
- ✓ Scalar product $\langle \psi_{1,free} | \psi_{1,cent} \rangle \sim 0.95$: weak variations.

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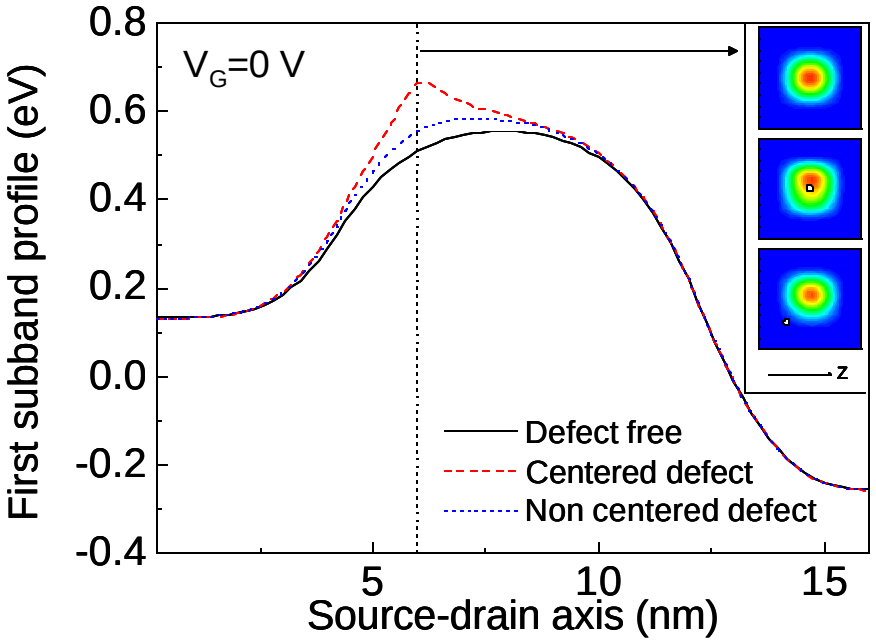
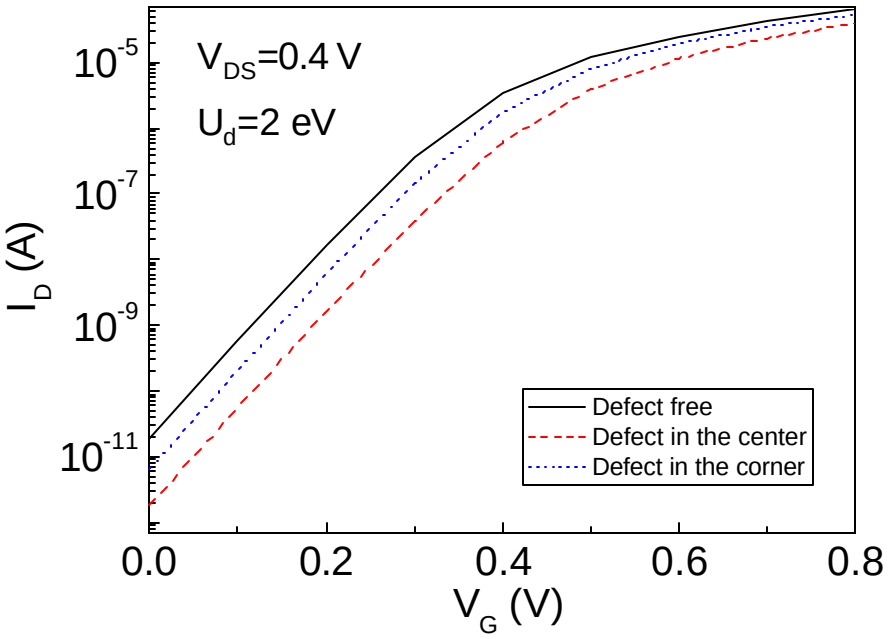
Simulation results

- First subband profile and current characteristics:





- ✓ Defect in the corner: weak influence on the subband profile.
- ✓ Defect free: highest current.
- ✓ Centered defect: lowest current.
- ✓ Defect in the corner: intermediate behavior: current decrease of 50%.
- ✓ Variation of the subthreshold slope.

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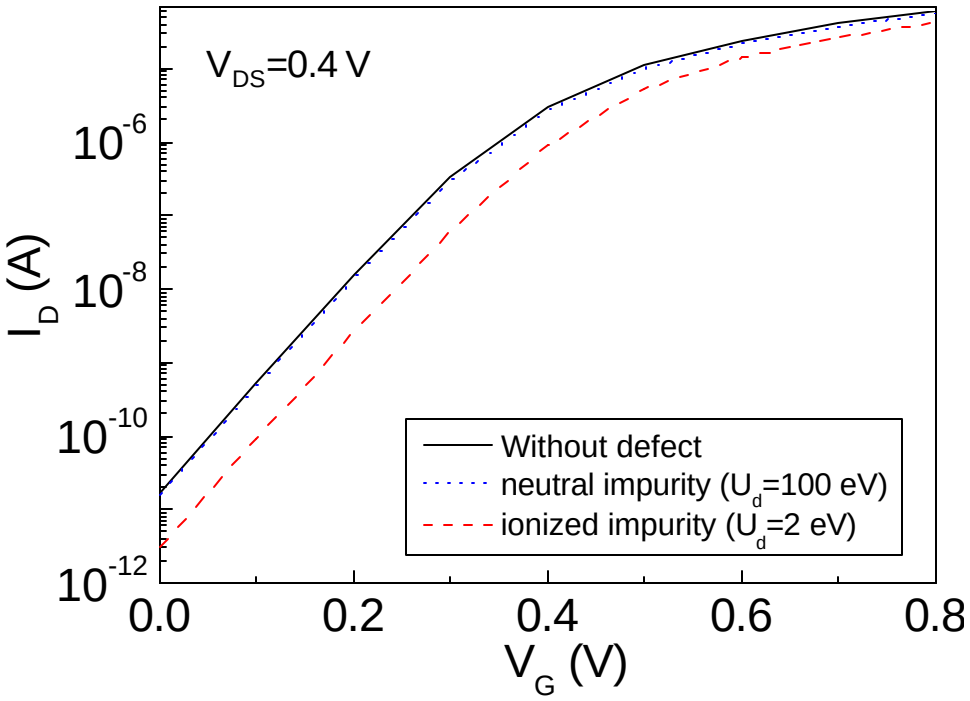
Simulation results

- Influence of Coulomb potential:



- ✓ On-site potential defect does not affect the total current.
- ✓ Coulombic potential has the most significant impact.
- ✓ Electrons can be transmitted through the unperturbated neighboring atoms.

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Conclusion

- Modeling of electron-ion interaction based on the NEGF formalism.
- Study of the effect the acceptor impurity in terms of physical properties.
- Centered impurity involves a significant degradation of the current.
- Not only a shift of the current but rather a subthreshold slope variation.
- The Coulomb potential has a prevalent rule compared to the on-site potential of the impurity.
- Treatment of donor impurities in source and drain.