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Quantum Transport Framework for Highly Conductive δ-layer Systems

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National Nuclear Security Administration

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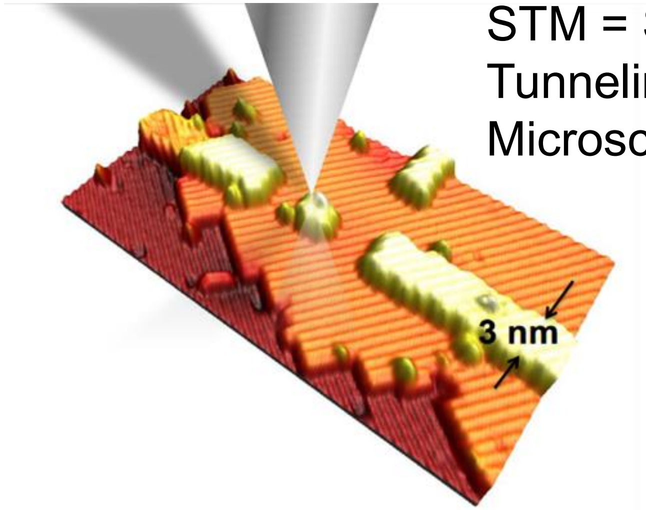
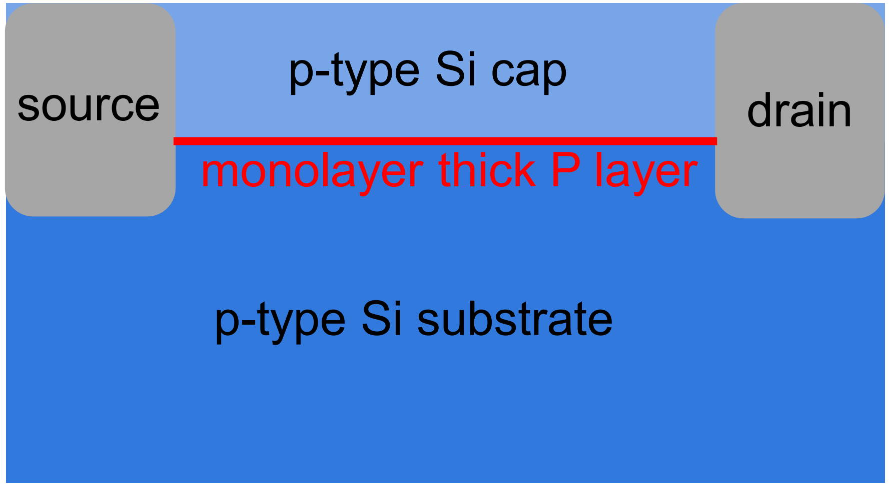
APAM Technology and δ-Layer Systems?

Atomic Precision Advanced Manufacturing (APAM)



STM = Scanning Tunneling Microscope



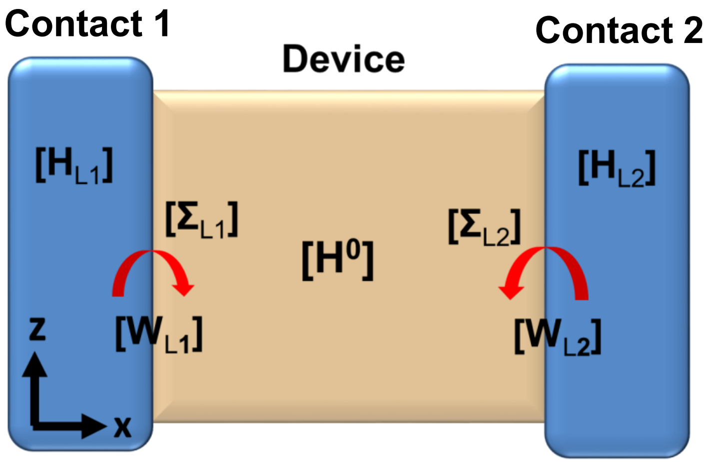
Si: P δ-layer nanodevice

- ❑ **APAM** is a process of area-selective dopant incorporation at the atomic scale
- ❑ High potential for **quantum computing** and **advanced microelectronic devices**

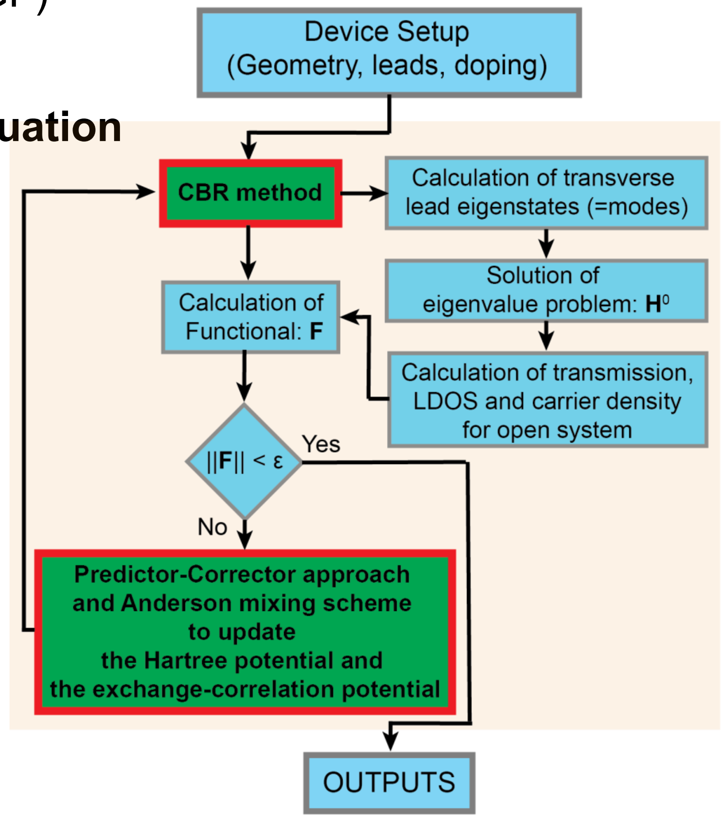
Open-system Quantum Transport Framework

Our quantum transport simulator is based on **Non-Equilibrium Green's function** (NEGF) formalism with

- **Fully charge self-consistent solution of Poisson-open system Schrödinger equation**
- **Single-band (Γ valley) effective mass approximation**
- Contact Block Reduction (CBR) method for fast numerical efficiency
- Predictor-corrector approach and Anderson mixing scheme



Quantum transport simulator



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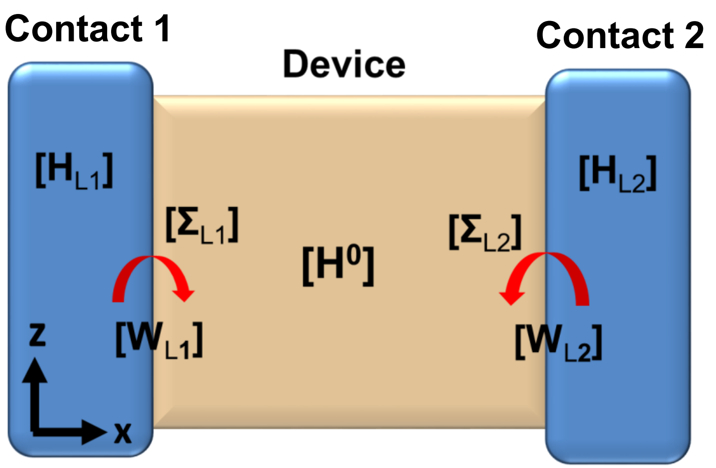
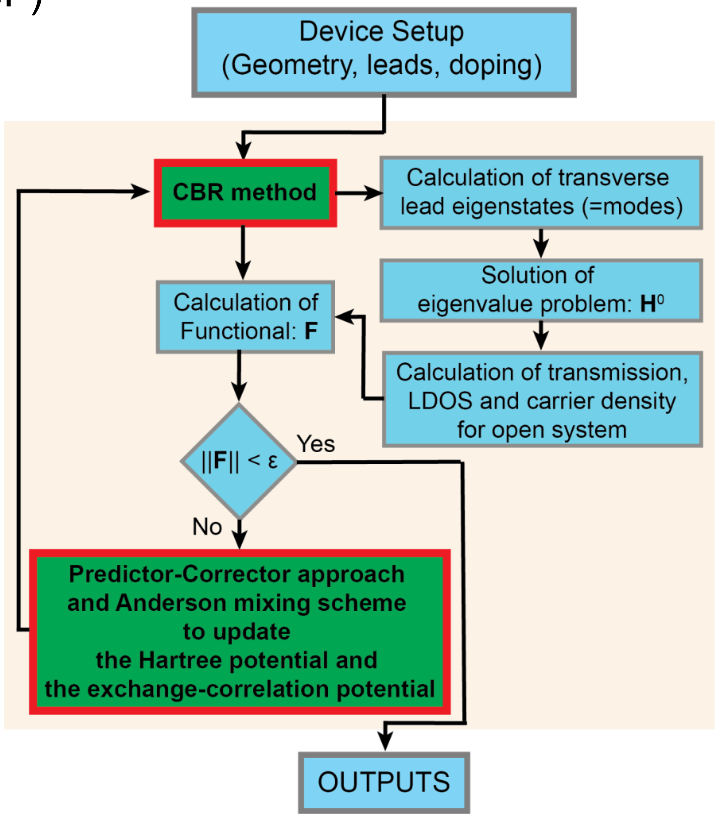


Quantum transport simulator



- D. Mamaluy *et al.,* J. Appl. Phys., vol. 93, no. 8, p. 4628-4633, 2003.
- D. Mamaluy *et al.* Phys. Rev. B, vol. 71, p. 245321, 2005.

Non-Equilibrium Green Function

- **Current from leads λ to λ'**

$$J_{\lambda\lambda'} = \frac{2e}{h}\int T_{\lambda\lambda'}(E)(f_\lambda(E) - f_{\lambda'}(E))dE$$

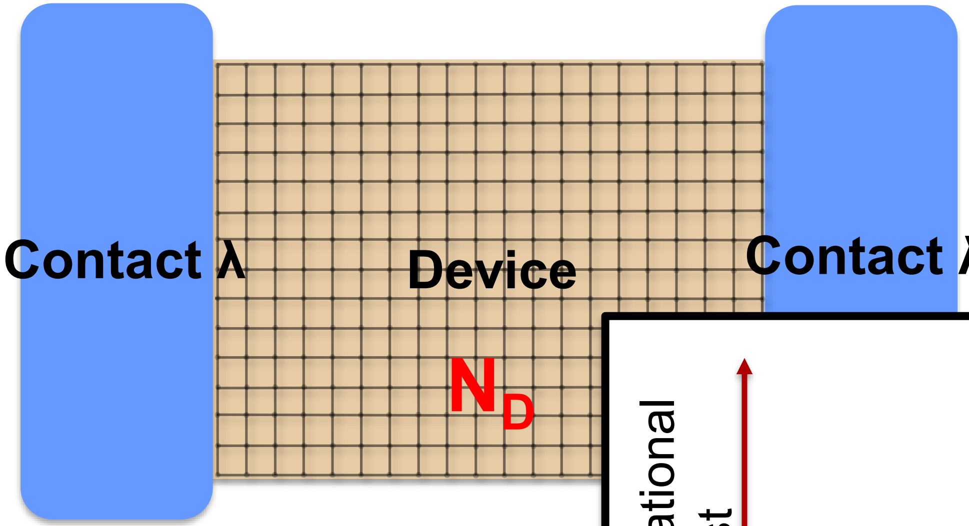
$$T_{\lambda\lambda'}(E) = \mathrm{Tr}\left[\boxed{\boldsymbol{\Gamma}_\lambda \boldsymbol{G}_D \boldsymbol{\Gamma}_{\lambda'} \boldsymbol{G}_D^\dagger}\right]$$

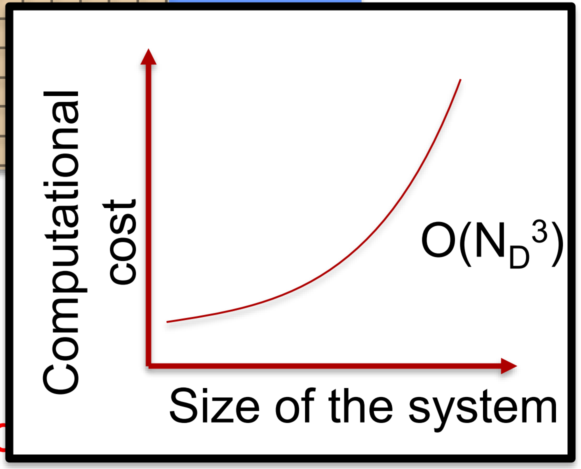
Self-energy matrix of lead

$$\boldsymbol{\Gamma}_\lambda = i(\boxed{\boldsymbol{\Sigma}_\lambda - \boldsymbol{\Sigma}_\lambda^\dagger})$$

Open-device Hamiltonian matrix

$$\boldsymbol{G}_D = \boxed{[\boldsymbol{I} - \boldsymbol{G}_D^0 \sum_{\lambda=\lambda_1}^{\lambda_L} \boldsymbol{\Sigma}_\lambda]}^{-1}\boldsymbol{G}_D^0$$ Dyson ec





- **Electron density**

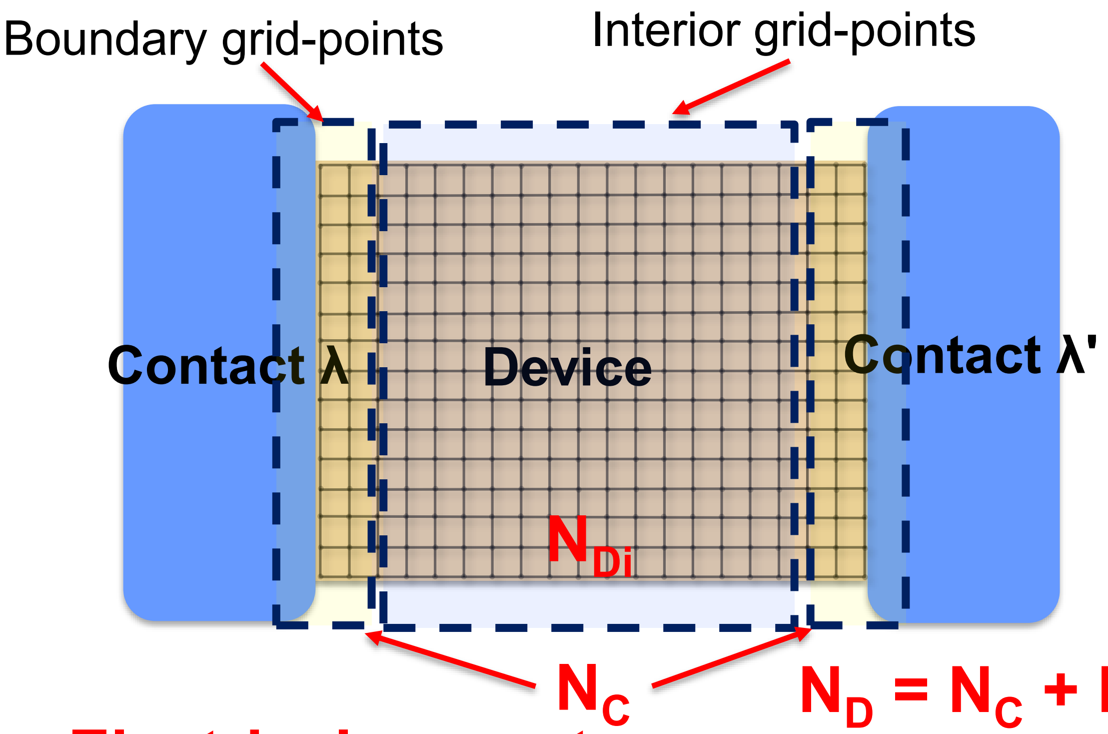
$$\boldsymbol{\rho}(\boldsymbol{r}_i) = \sum_\lambda \int_{-\infty}^{\infty} \boldsymbol{\rho}_\lambda(\boldsymbol{r}_i, E) f_\lambda(E) dE$$

$$\boldsymbol{\rho}_\lambda(\boldsymbol{r}_i, E) = \frac{1}{2\pi}\boxed{\boldsymbol{G}_D \boldsymbol{\Gamma}_\lambda \boldsymbol{G}_D^\dagger}$$

$$\boxed{\boldsymbol{G}_D^0} = [\boxed{\boldsymbol{E}^+ - \boldsymbol{H}_D^0}]^{-1} = \sum_\alpha \frac{|\phi_\alpha\rangle\langle\phi_\alpha|}{E^+ - E_\alpha}$$

(N_D × N_D)

Contact Block Reduction Method



$$\boldsymbol{H}_D = \begin{pmatrix} \boxed{\boldsymbol{H}_C} & \boxed{\boldsymbol{H}_{CD_i}} \\ \boxed{\boldsymbol{H}_{D_iC}} & \boxed{\boldsymbol{H}_{D_i}} \end{pmatrix}$$

$(N_D \times N_D)$ $(N_C \times N_C)$ $(N_C \times N_{Di})$ $(N_{Di} \times N_{Di})$

$$\boldsymbol{G}_D = \begin{pmatrix} \boxed{\boldsymbol{G}_C} & \boxed{\boldsymbol{G}_{CD_i}} \\ \boxed{\boldsymbol{G}_{D_iC}} & \boxed{\boldsymbol{G}_{D_i}} \end{pmatrix}$$

$$\boldsymbol{\Sigma} = \sum_{\lambda=\lambda_1}^{\lambda_L} \boldsymbol{\Sigma}_\lambda = \begin{pmatrix} \boxed{\boldsymbol{\Sigma}_C} & \boxed{\mathbf{0}} \\ \boxed{\mathbf{0}} & \boxed{\mathbf{0}} \end{pmatrix}$$

$N_D = N_C + N_{Di}$ $N_D > N_{Di} >>> N_C$!!

- **Electrical current:**

$$J_{\lambda\lambda'} = \frac{2e}{h}\int T_{\lambda\lambda'}(E)(f_\lambda(E) - f_{\lambda'}(E))dE, \quad T_{\lambda\lambda'}(E) = \mathrm{Tr}\left(\boxed{\boldsymbol{\Gamma}_{C_\lambda}\boldsymbol{G}_C\boldsymbol{\Gamma}_{C_{\lambda'}}\boldsymbol{G}_C^\dagger}\right), \quad \boldsymbol{G}_C = \boxed{[\boldsymbol{I} - \boldsymbol{G}_C^0\boldsymbol{\Sigma}_C]^{-1}\boldsymbol{G}_C^0}$$

- **Electron density:**

$$\rho(\boldsymbol{r}_i) = \int_{-\infty}^{\infty} \Xi(E) f_\lambda(E)dE, \quad \Xi(E) = \frac{1}{2\pi}\frac{\mathrm{Tr}\left[\boxed{\boldsymbol{B}_C^{-1}\boldsymbol{\Gamma}_C\boldsymbol{B}_C^{-1\dagger}}\right]}{(E^+ - E_\alpha)(E^- - E_\alpha)}, \quad \boldsymbol{B}_C = \boxed{\boldsymbol{1}_C - \boldsymbol{\Sigma}_C\boldsymbol{G}_C^0}$$

$(N_C \times N_C)$

Open-system Quantum Transport Framework

Our quantum transport simulator is based on **Non-Equilibrium Green's function** (NEGF) formalism with

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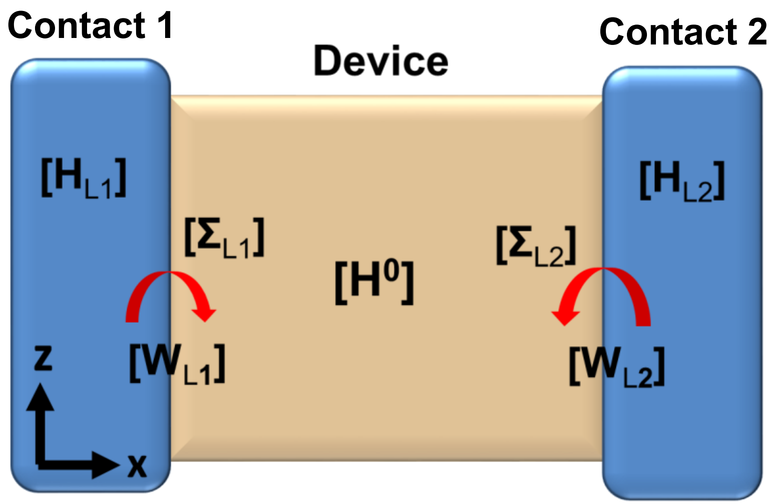
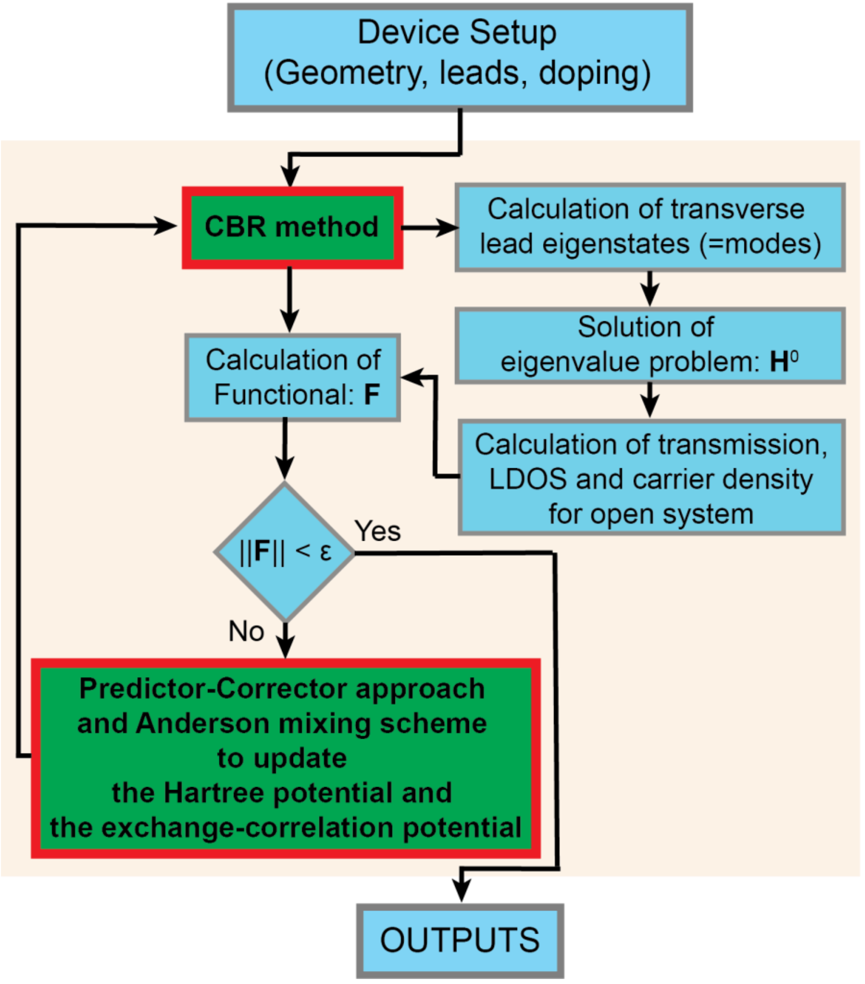
- Contact Block Reduction (CBR) method [1,2] for fast numerical efficiency
- **Predictor-corrector approach and Anderson mixing scheme**

X. Gao *et al*., J. Appl. Phys., vol. 115, no. 13, p. 133707, 2014.

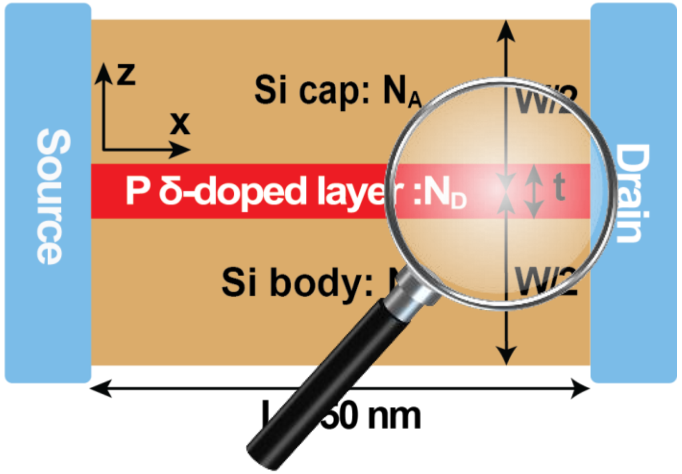


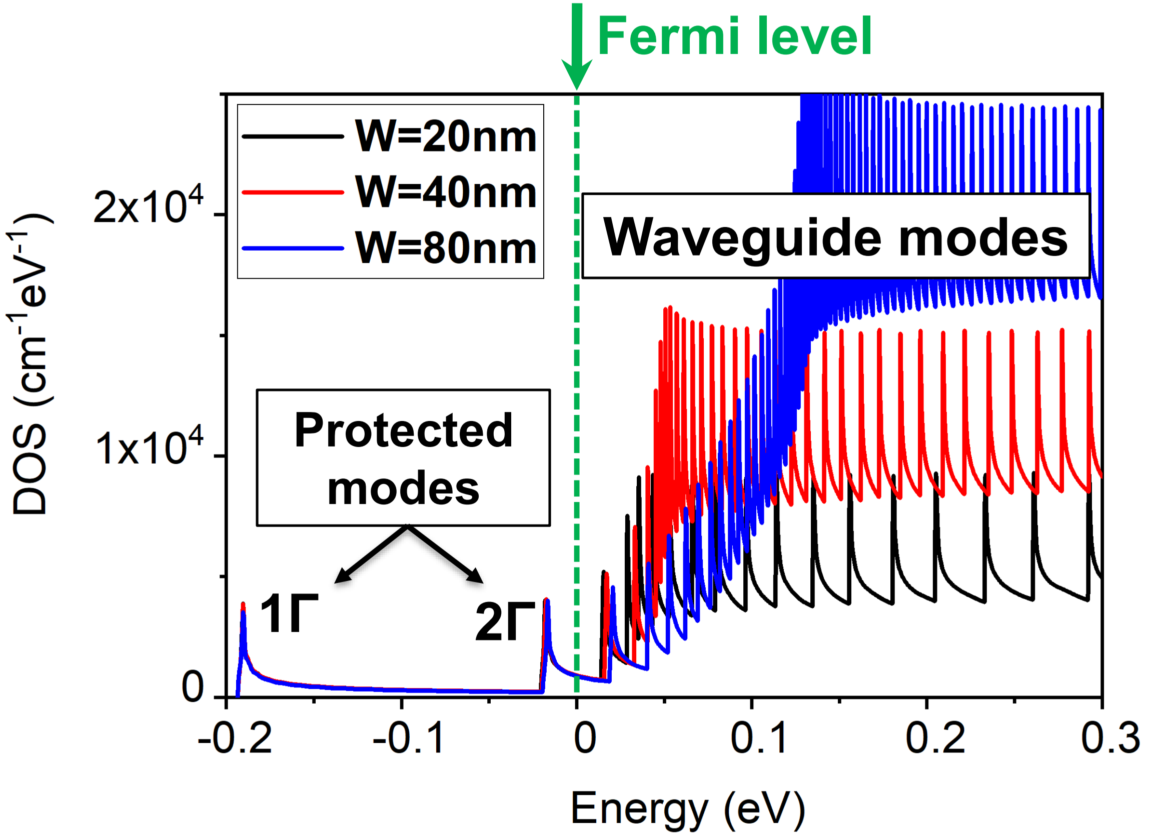
Quantum transport simulator



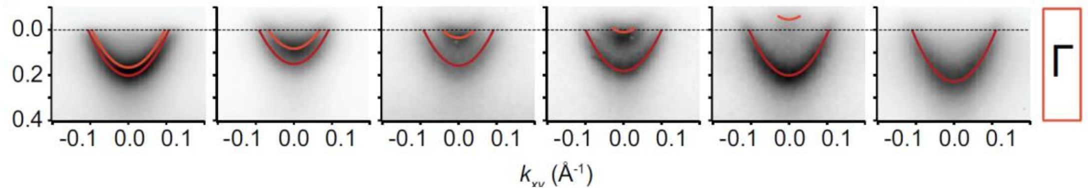
Prediction of Shallow Sub-bands

$N_D=10^{14}$ cm^{-2}, $N_A=10^{17}$ cm^{-3}, t=0.2 nm





- Our open-system quantum simulations **predict shallow sub-bands**
- Below the Fermi energy level the states are "protected" (independent of encapsulation depth).

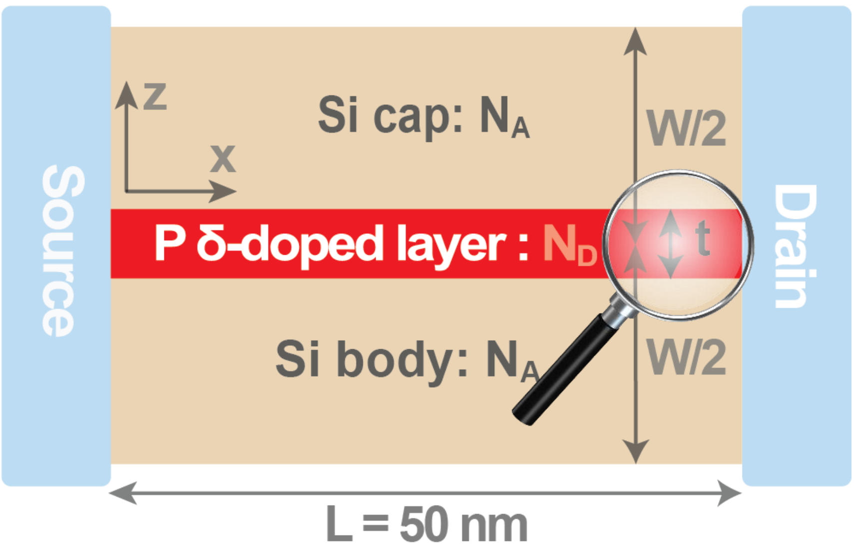


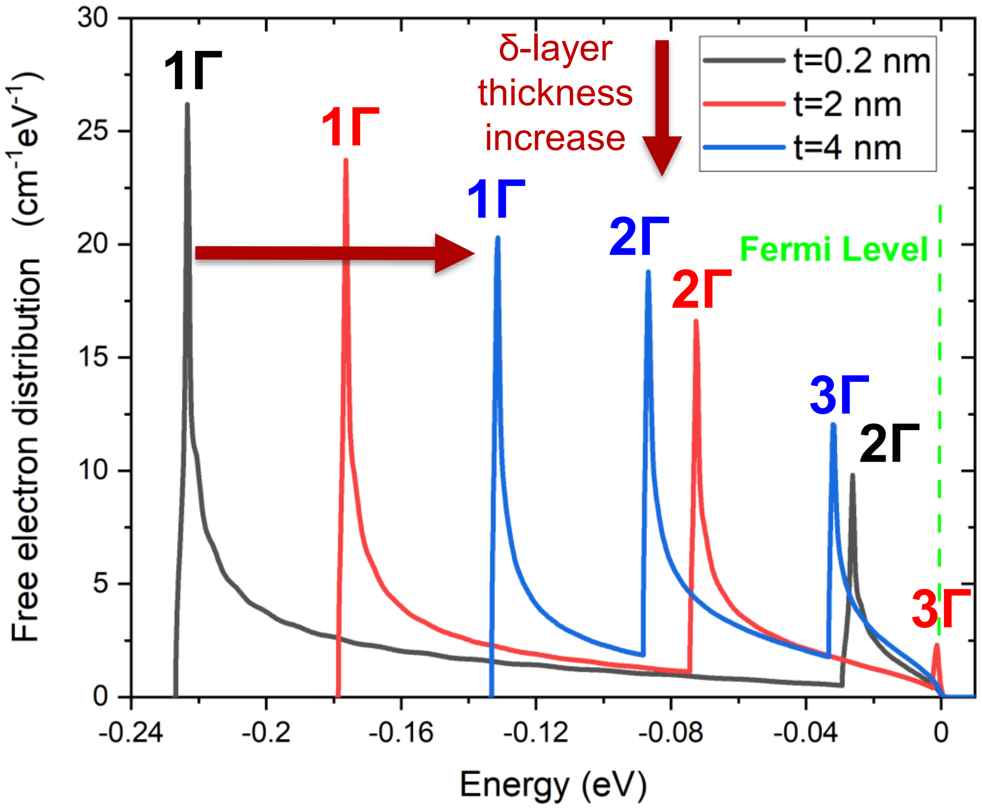
A. J. Holt *et al.*, Phys. Rev. B, vol. 101, p. 121402(R), 2020

How are these conductive sub-bands influenced by the thickness of δ-layer?

Influence of the δ-layer thickness

N_D=1.2×10^{14} cm^{-2}, N_A=10^{17} cm^{-3}, W=40nm





- For a fixed sheet doping, the increment of the delta-layer thickness increases the number of modes, but decreases the energy splitting between them

Influence of the δ-layer thickness

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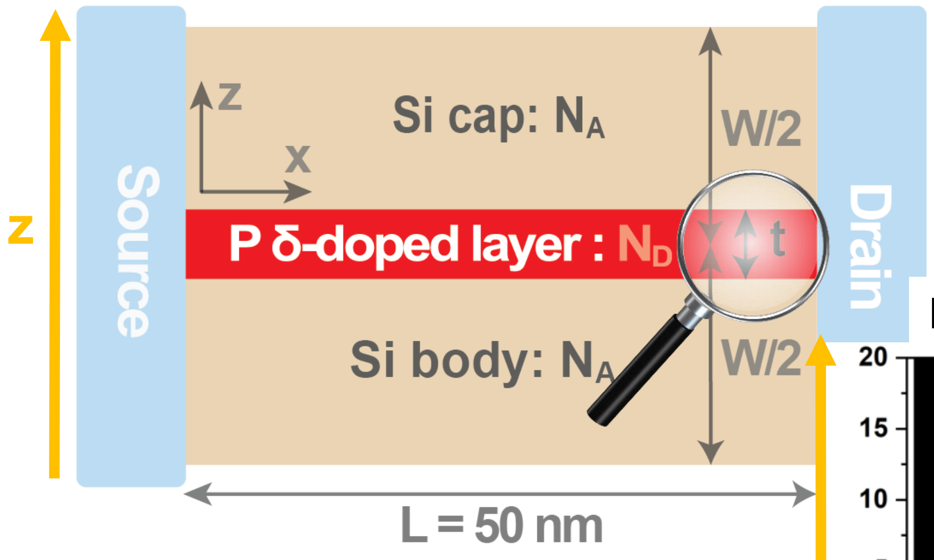
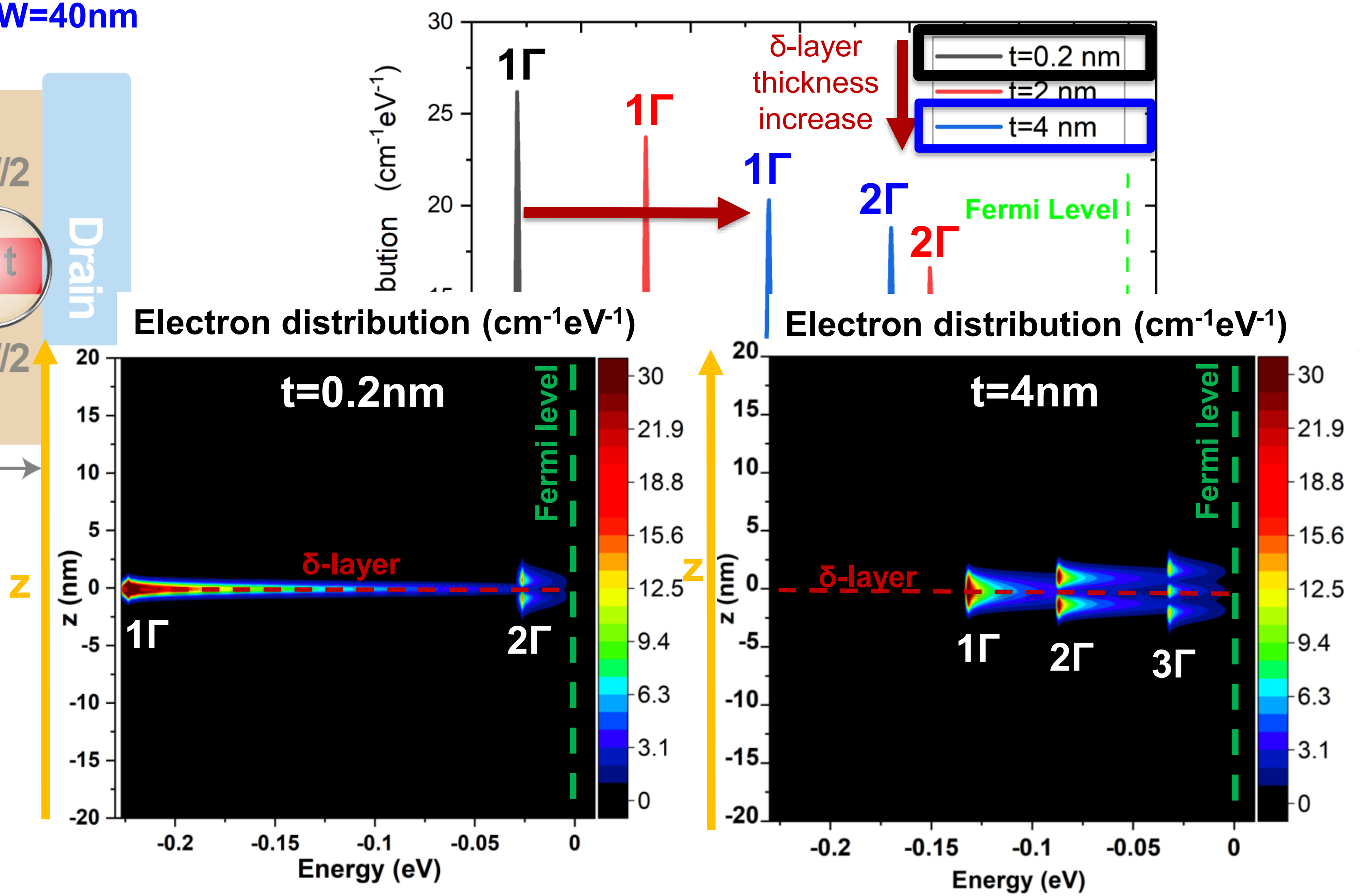
N_D=1.2×10^{14} cm^{-2}, N_A=10^{17} cm^{-3}, W=40nm





- **Space quantization** of the modes: they are separated in space and with distinct structure

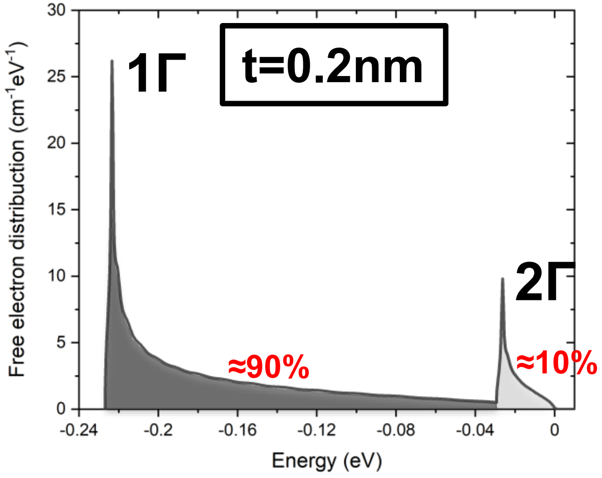
Electron contribution on the current

- **Dissimilar contribution of the conductive sub-bands on the electronic current**

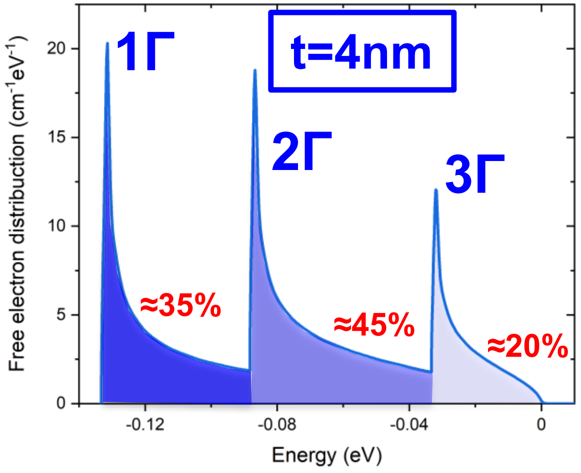
Sharp doping profile
= strong confinement potentials

Smooth doping profile
= weak confinement potentials

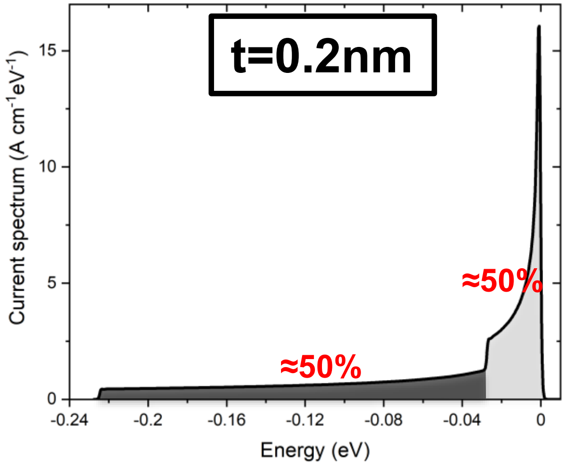
Free electron distribution

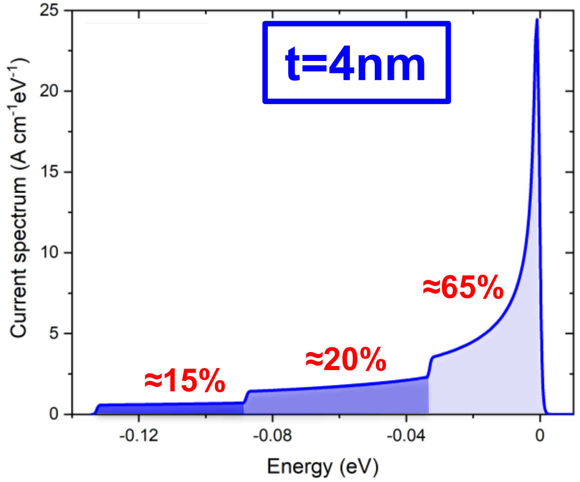


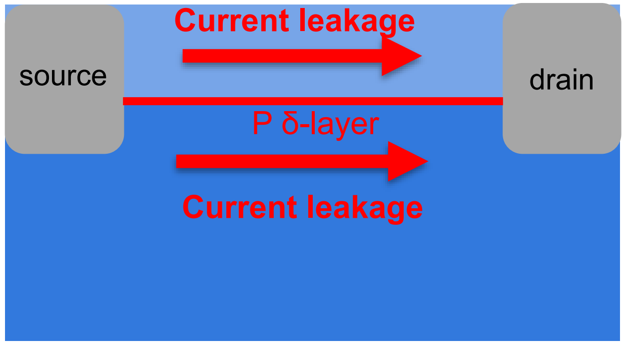
VS.



Current spectrum





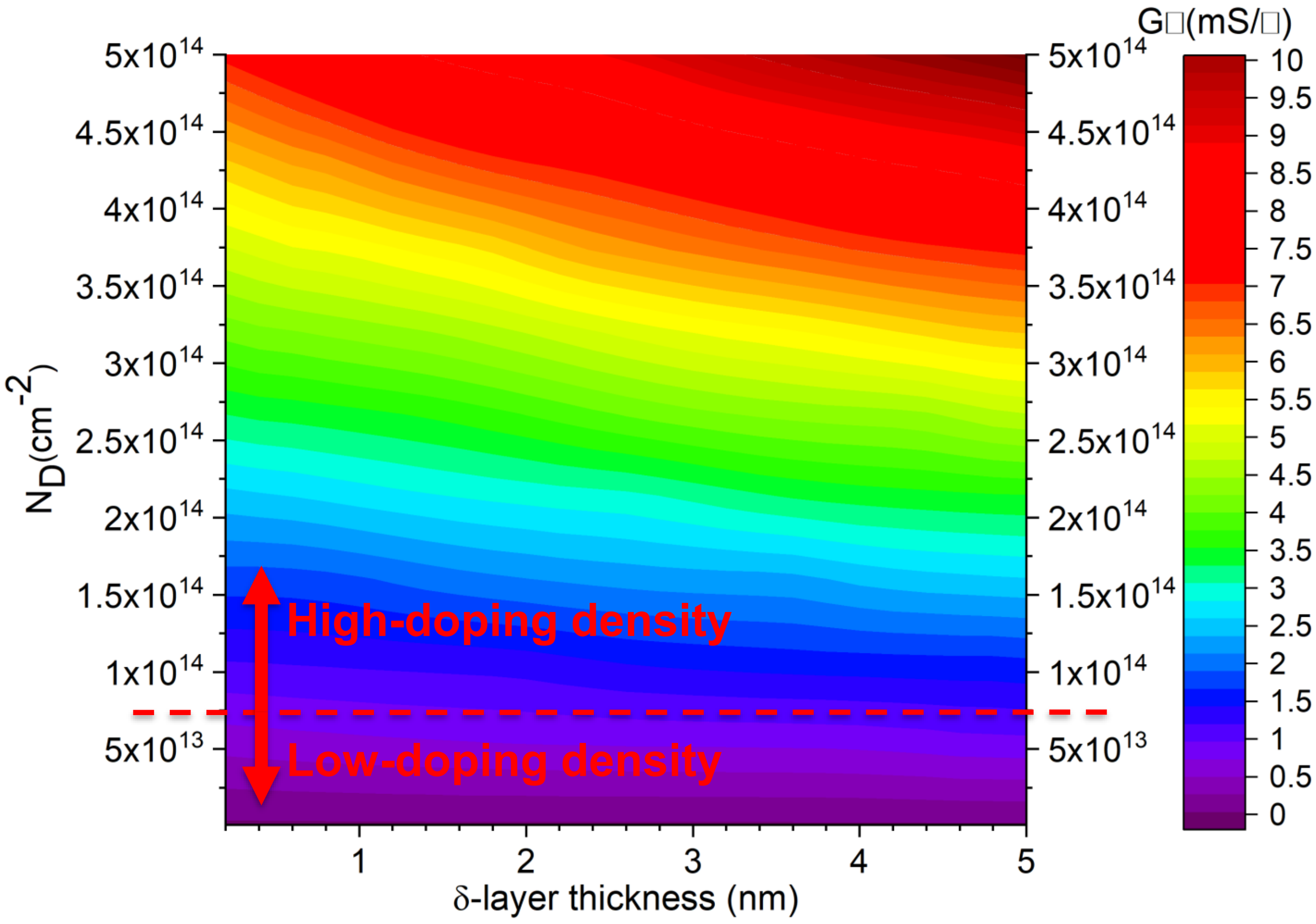


- Sharp doping profile reduces the current leakage

N_D=1.2×10^{14} cm^{-2}, N_A=10^{17} cm^{-3}, W=40nm

Sheet conductance for Si: P δ-layer wires

- **Our simulations predicts a quantum thickness dependence on the sheet conductance**



Mamaluy, D *et al*. (2020) "Revealing Quantum Effects in Highly Conductive δ-layer Systems" Submitted to Communications Physics (2021)

Summary

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- ❑ Presented an **efficient quantum open-system transport framework** for highly conductive δ-layer systems

- ❑ Predicted the **conductive shallow sub-bands** observed experimentally, and evaluated how these conductive sub-bands are influenced by **thickness of the δ-layer**

- ❑ Shown **quantum thickness dependence** on the conductive properties for δ-layer systems


thank you
gracias
merci
obrigado
danke
謝謝
ngiyabonga
teşekkür ederim
go raibh maith agat
mochchakkeram
dziękuję
bedankt
sukriya
kop khun krap
terima kasih
grazie
arigatô
dakujem
takk
taiku
tapadh leat
dank je
спасибо
Баярлалаа
рахмат
мерси
хвала
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спасибі
ありがとう
감사합니다
ευχαριστώ
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tanemirt
najis tuke
rahmat
kam sah hamnida
didi madloba
mèsi
dêkuji
sobodi

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