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Quantum transport in Si:P δ-layer wires

Juan P. Mendez, Denis Mamaluy, Xujiao (Suzey) Gao, Evan M. Anderson, DeAnna M. Campbell, Jeffrey A. Ivie, Tzu-Ming Lu, Scott W. Schmucker, and Shashank Misra

jpmende@sandia.gov

Sandia National Laboratories, Albuquerque, New Mexico

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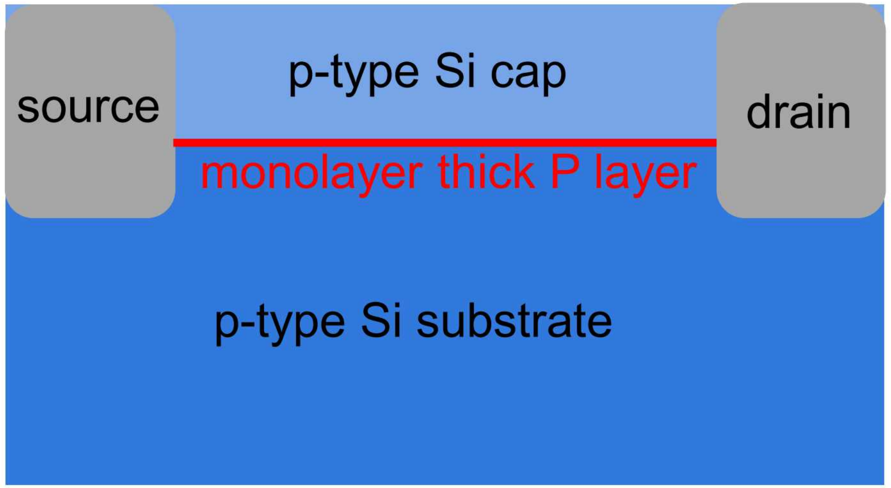
What is a Si: P δ-layer nanodevice?



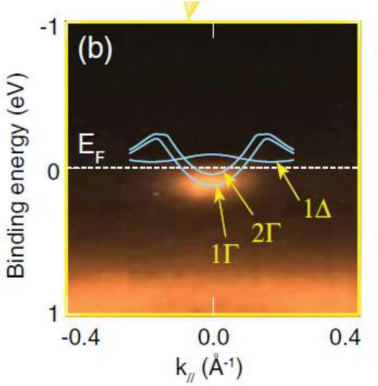
Schematic model of a Si: P δ-layer nanodevice

- High potential for quantum computing and advanced microelectronic devices
- The current advances to place dopants with atomic precision using hydrogen lithography

Atomic Precision Advanced Manufacturing (APAM)

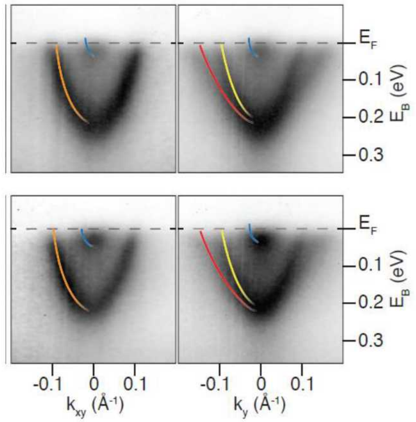
Conductive shallow sub-bands

J. A. Miwa, et al.,
*Nano Letters 14, 1515 (**2014**)*



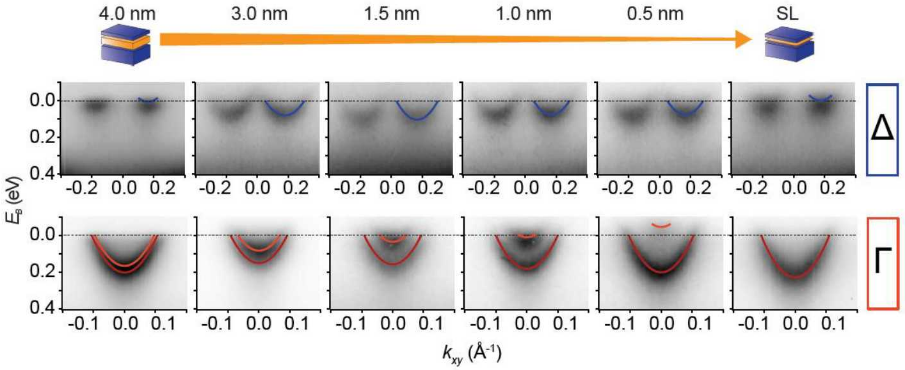
First observation of conductive shallow sub-bands (1Γ and 2Γ)

F. Mazzola, et al.,
*npj Quantum Materials 5 (**2020**)*

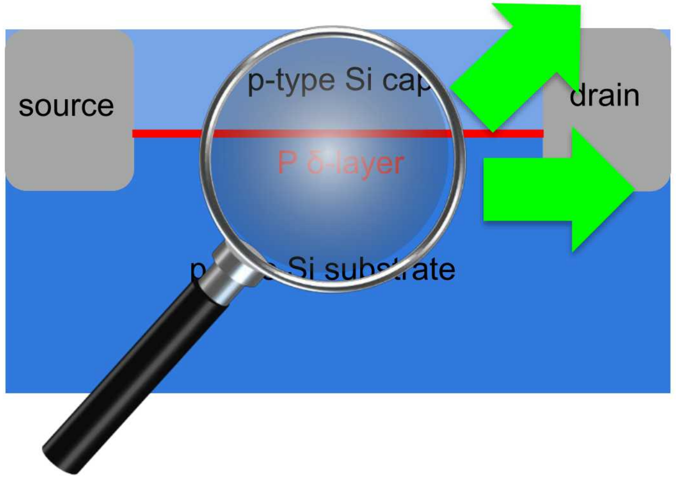


First observation of three sub-bands (1Γ, 2Γ and 3Γ)

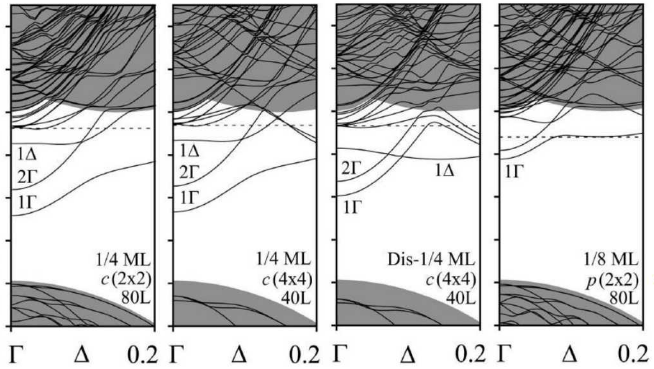
A. J. Holt, et al.,
*Phys. Rev. B 101, 121402 (**2020**)*



First observation of the Δ sub-band



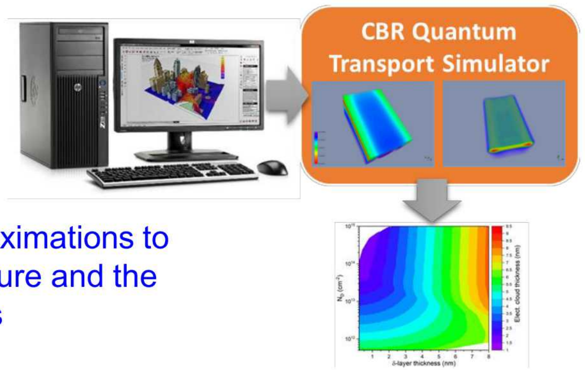
D. J. Carter, et al.,
*Phys. Rev. B 79, 033204 (**2009**)*



Study of the electronic structure of Si: P δ-layer systems using **DFT**

This Work

***Open-system* quantum transport treatment**



- Closed system approximations to study the band structure and the conductive properties

Closed systems vs. Open systems

Closed system BC

Open system BC

vs

- Extract the conductive properties from the additional (semi-)classical approximations (Drude or mobility-based)

$$J = e\, n_{2D}\; \mu\; E \sim n_{2D}$$

- Extract the conductive properties from the quantum flux

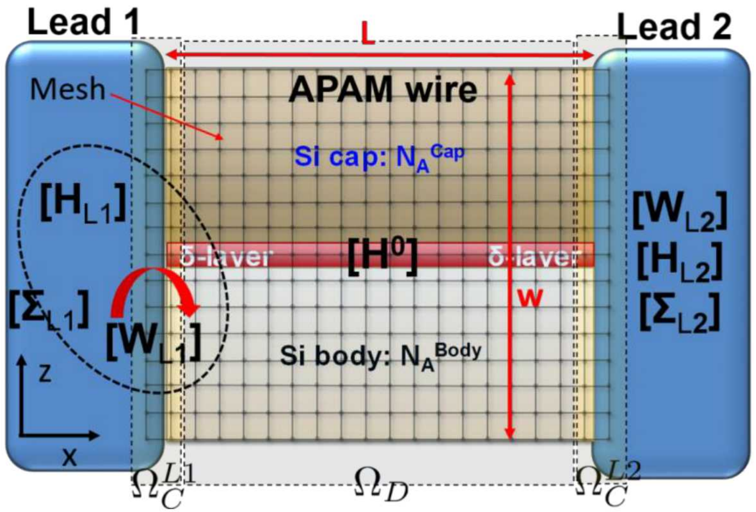
$$j \sim \Psi \nabla \Psi^* - \Psi^* \nabla \Psi$$

$$\boxed{\sigma = \frac{J}{\mathcal{E}}} \qquad \boxed{G = \sigma \frac{A}{L}}$$

Open-System Quantum Transport

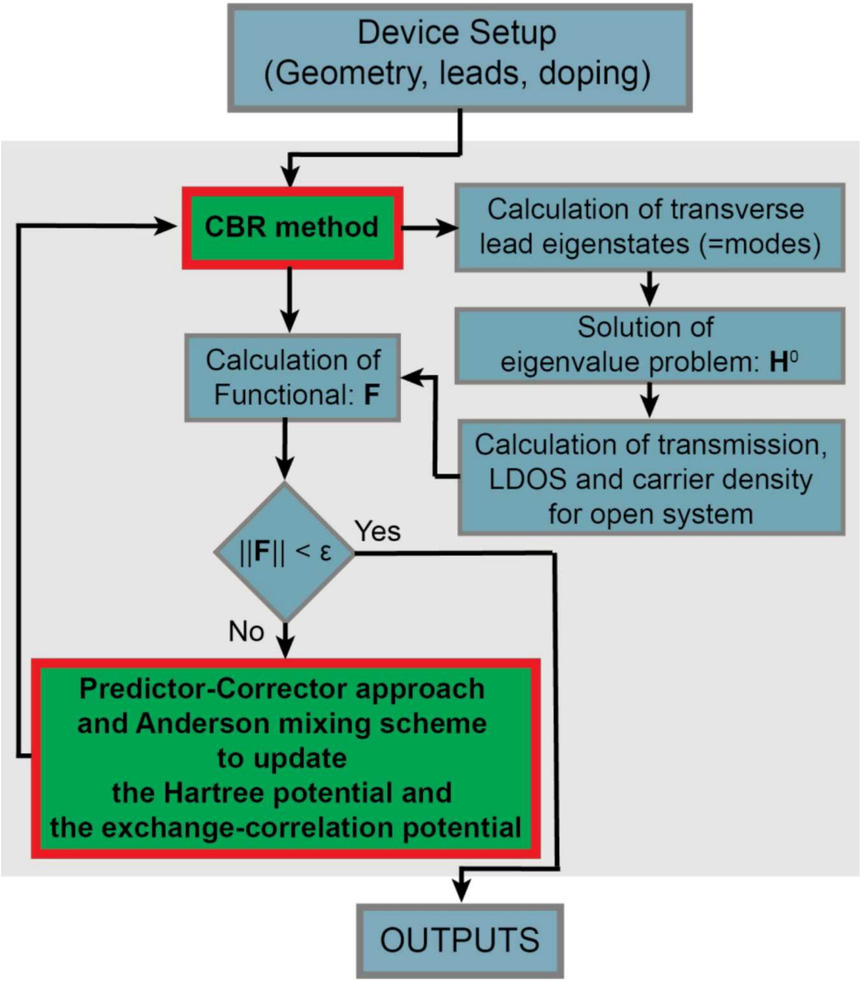
Our quantum transport simulator is based on **Non-Equilibrium Green's function** (NEGF) formalism with

- Fully charge self-consistent solution of Poisson-open system Schrödinger equation
- Single-band (Γ valley) effective mass approximation
- **Contact Block Reduction (CBR) method** [1,2] for fast numerical efficiency
- **Predictor-corrector approach** and **Anderson mixing scheme** [3]



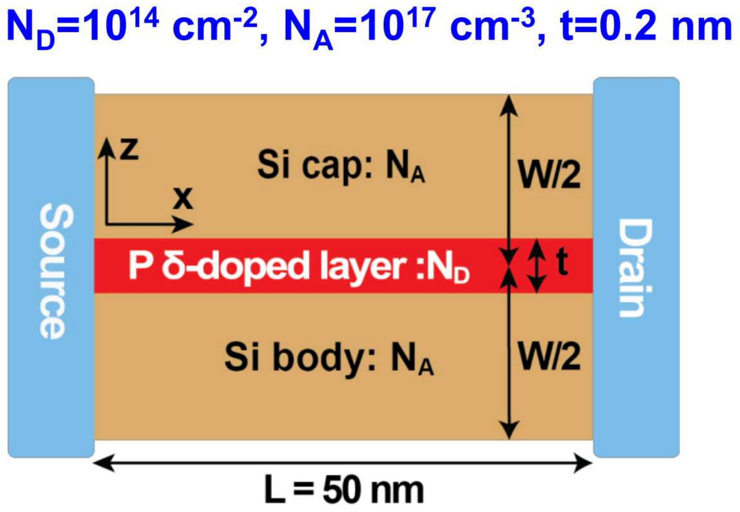
Simulations were done for the cryogenic temperature of **4 K**.

Quantum transport simulator

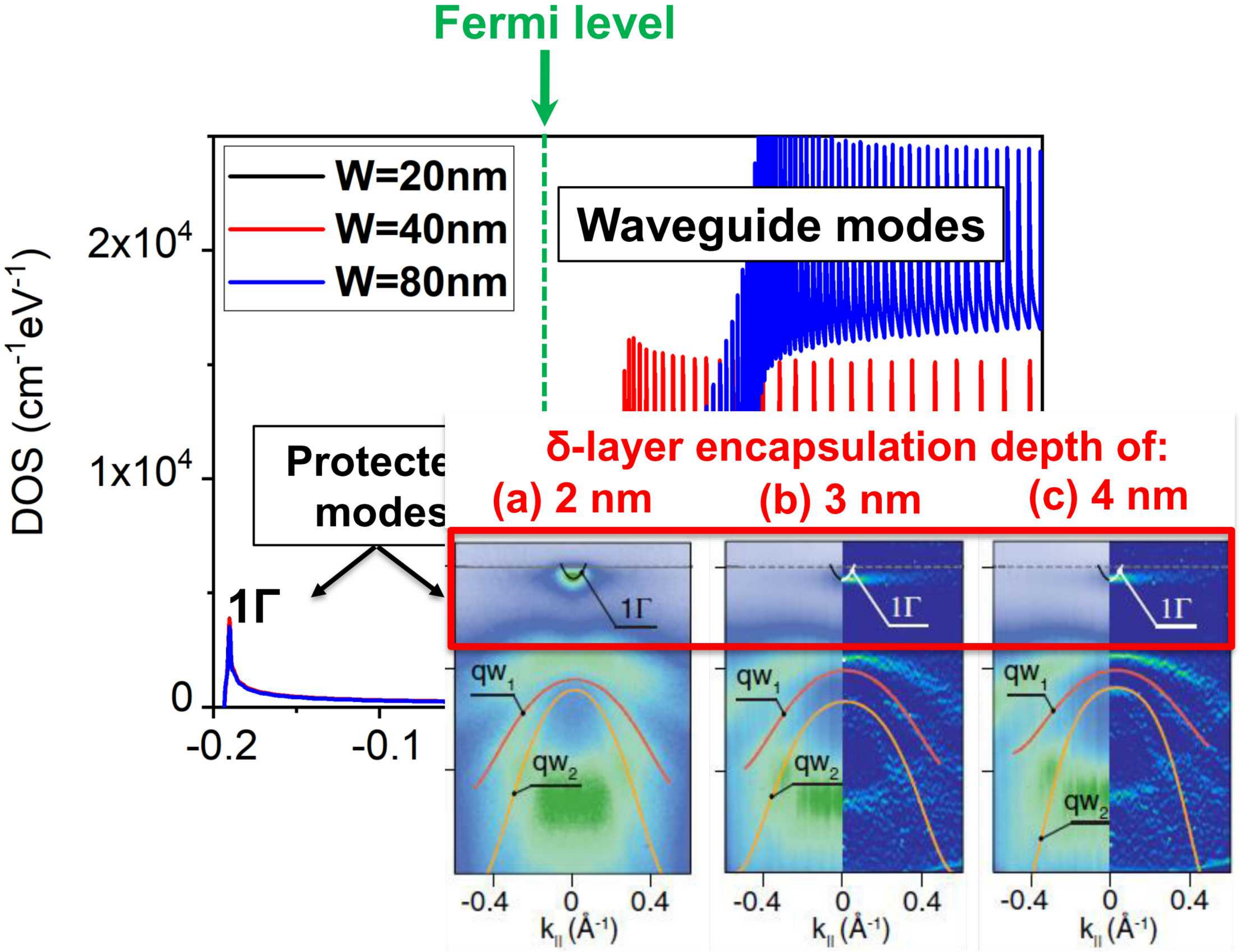


[1] D. Mamaluy *et al.*, J. Appl. Phys., vol. 93, no. 8, pp. 4628–4633, 2003.
[2] D. Mamaluy *et al.* Phys. Rev. B, vol. 71, p. 245321, 2005.
[3] X. Gao *et al.*, J. Appl. Phys., vol. 115, no. 13, p. 133707, 2014.

Prediction of Shallow Sub-bands



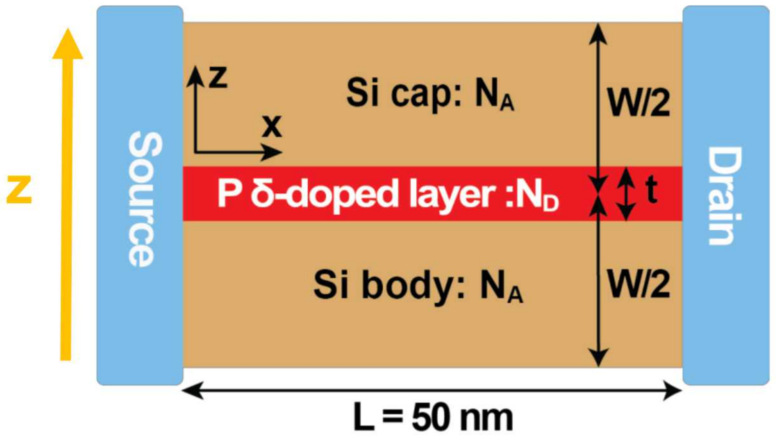
- Our open-system quantum simulations **predict shallow sub-bands**
- 1Γ sub-band is about 190 meV and 2Γ sub-band is about 20 meV below the Fermi level
- Below the Fermi energy level the states are "protected" (independent of encapsulation depth).



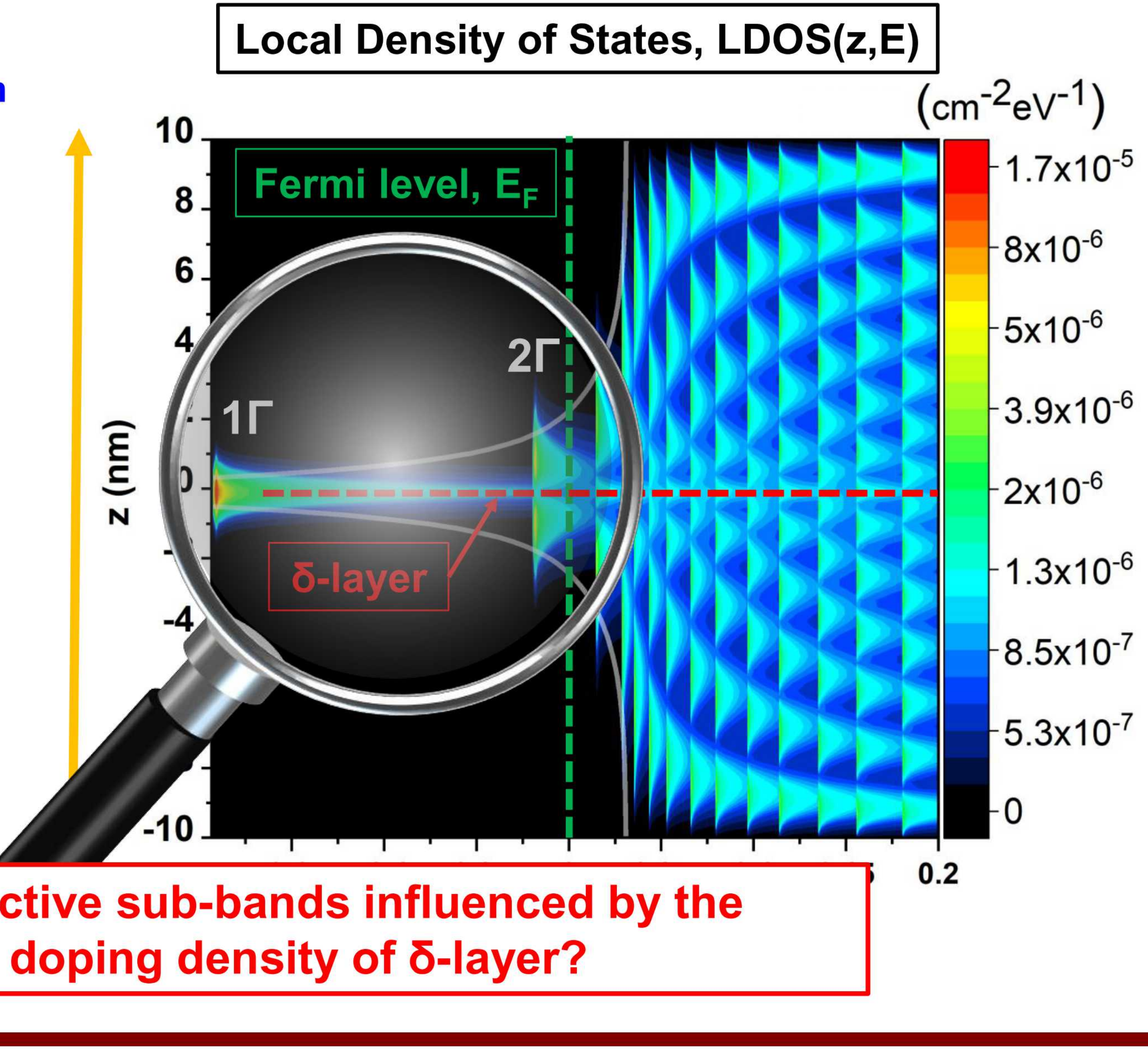
F. Mazzola, *et* al. Phys. Rev. Lett. 120, 046403, 2018

Si: P δ-layer conduction band structure

N_D=1.2x10^{14} cm^{-2}, N_A=10^{17} cm^{-3}, t=0.2 nm, W= 20 nm



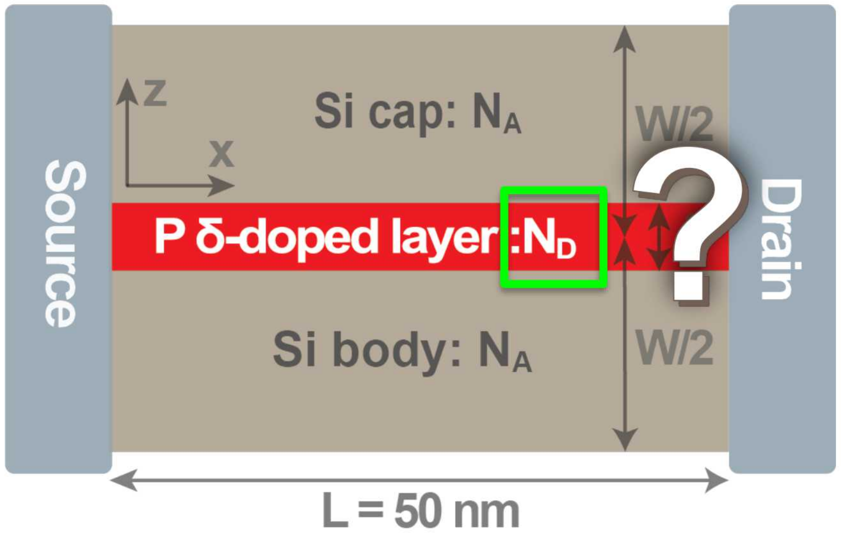
- **Space quantization** of the modes: they are separated in space and with distinct structure

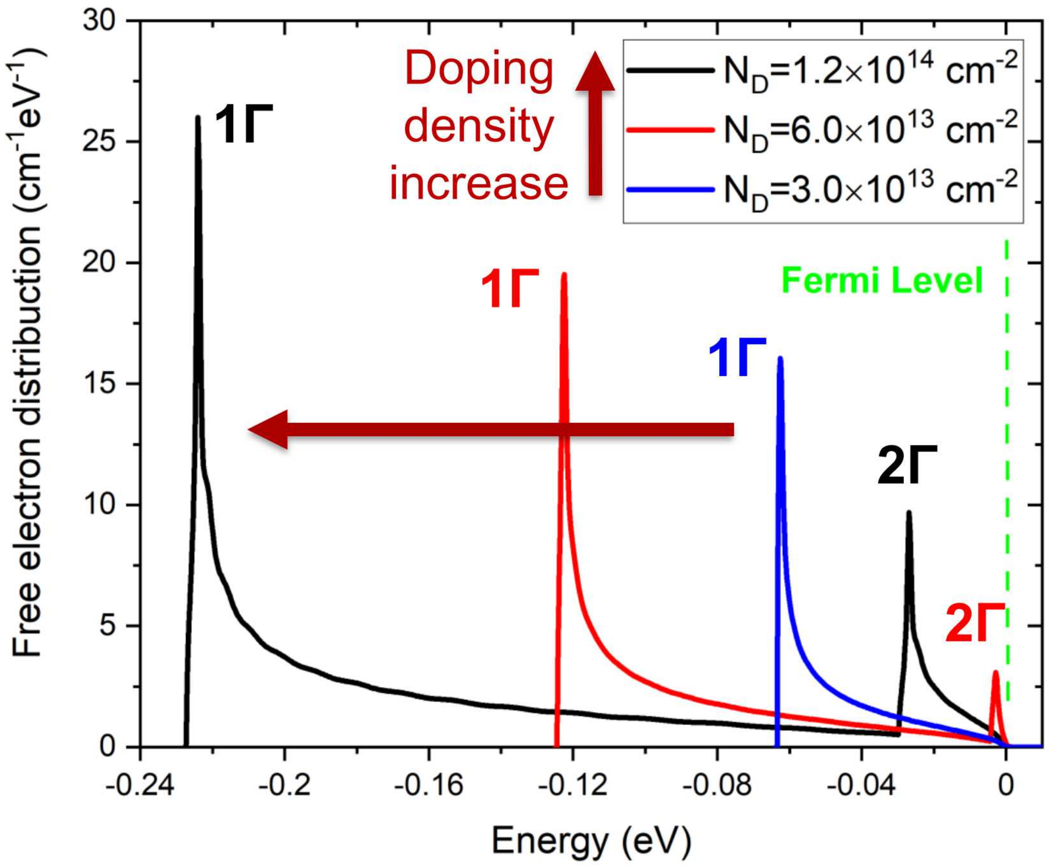


How are these conductive sub-bands influenced by the thickness and doping density of δ-layer?

Influence of δ-layer doping density

N_A=10^{17} cm^{-3}, t=0.2 nm, W=40 nm

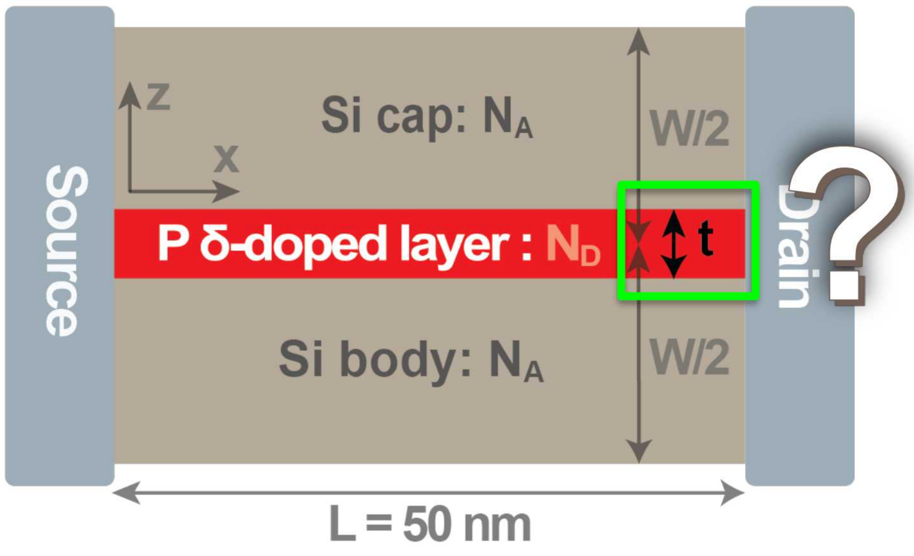


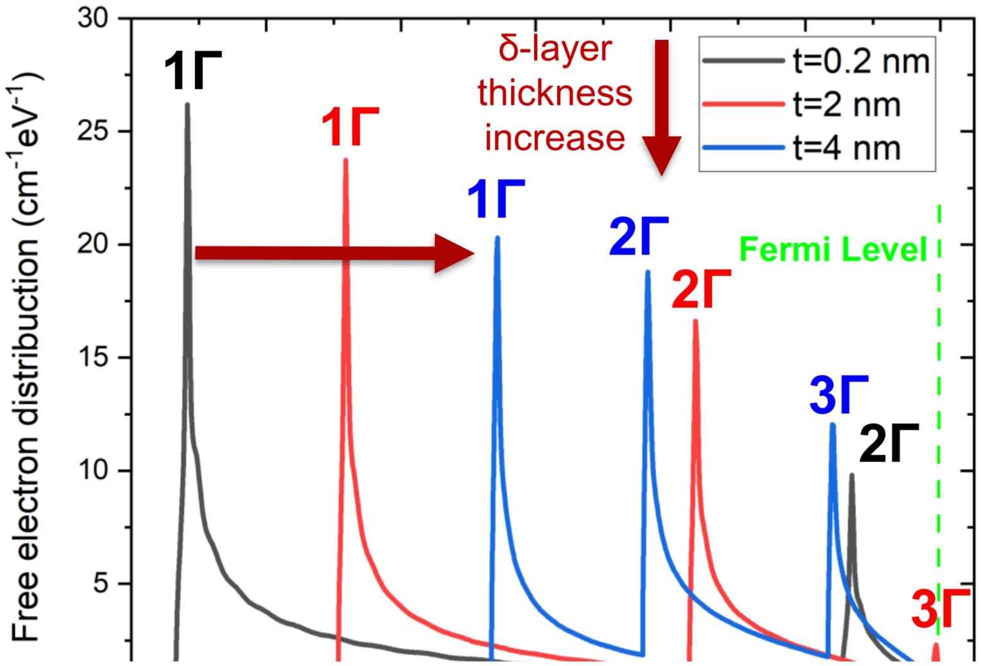


- For a fixed δ-layer thickness, the **increment of the sheet doping** N_D **increases the number of conducting modes**, as well as the **splitting energy** between them

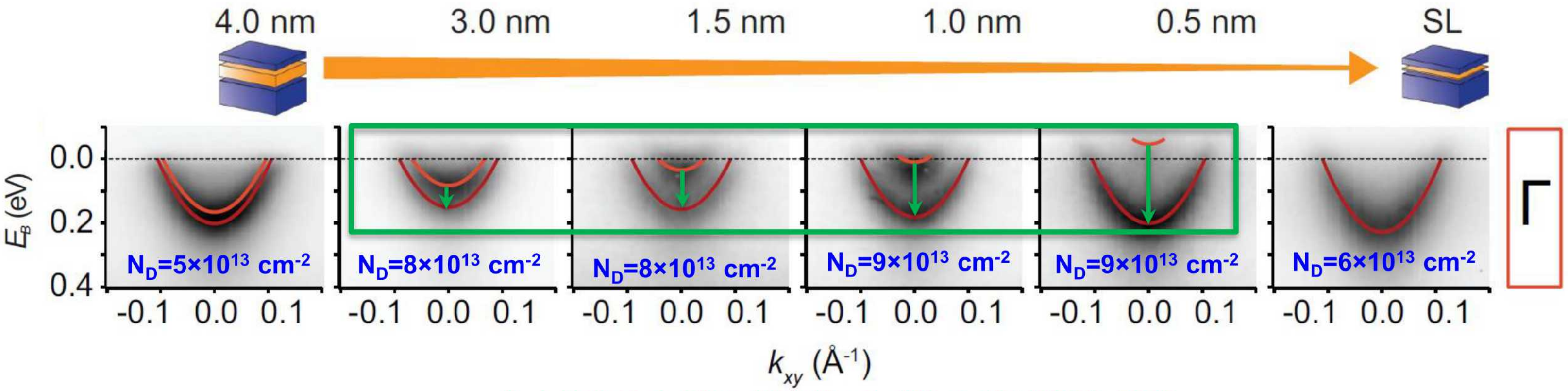
Influence of the δ-layer thickness

$N_D=1.2\times10^{14}$ 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



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

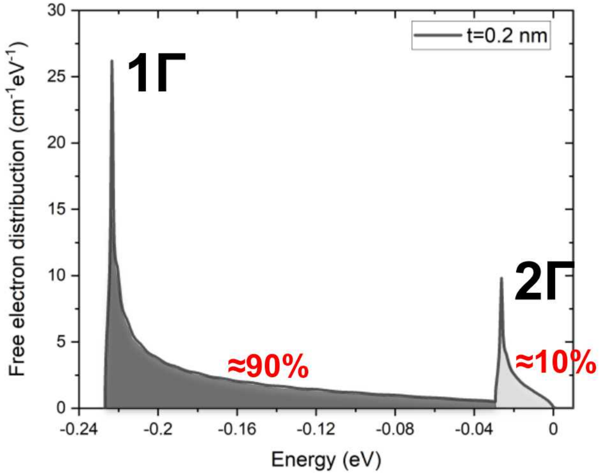
Electron contribution on the current

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

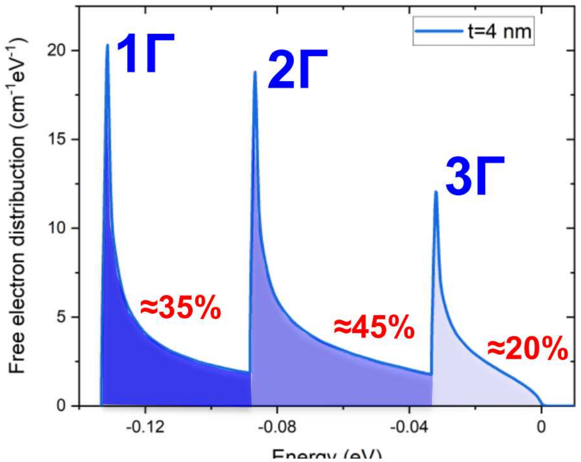
For strong confinement potentials = Sharp doping profile

For weak confinement potentials = Smooth doping profile

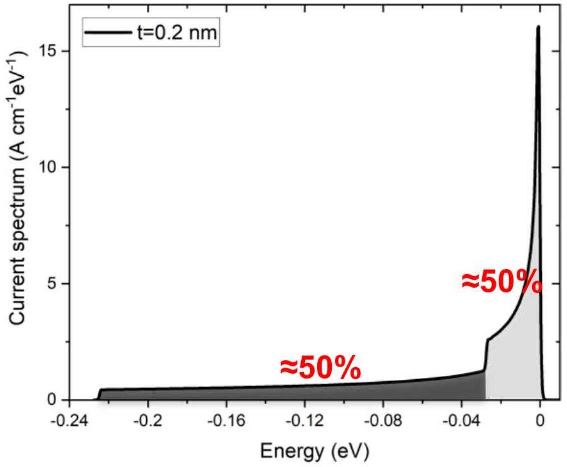
Free electrons distribution

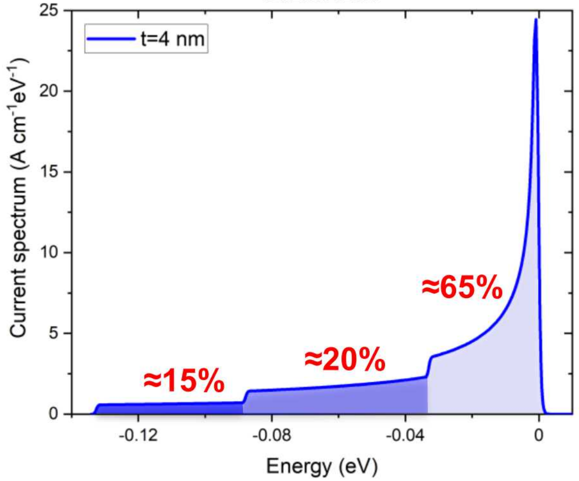


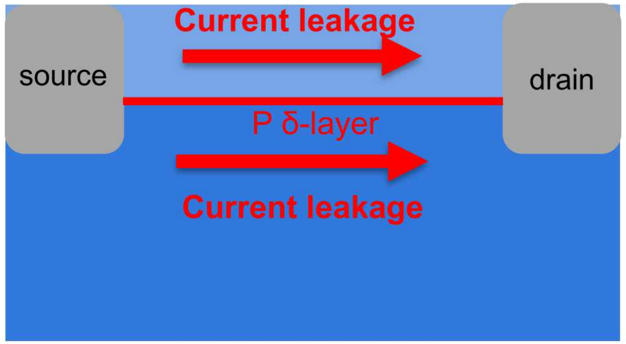
VS.



Current spectrum



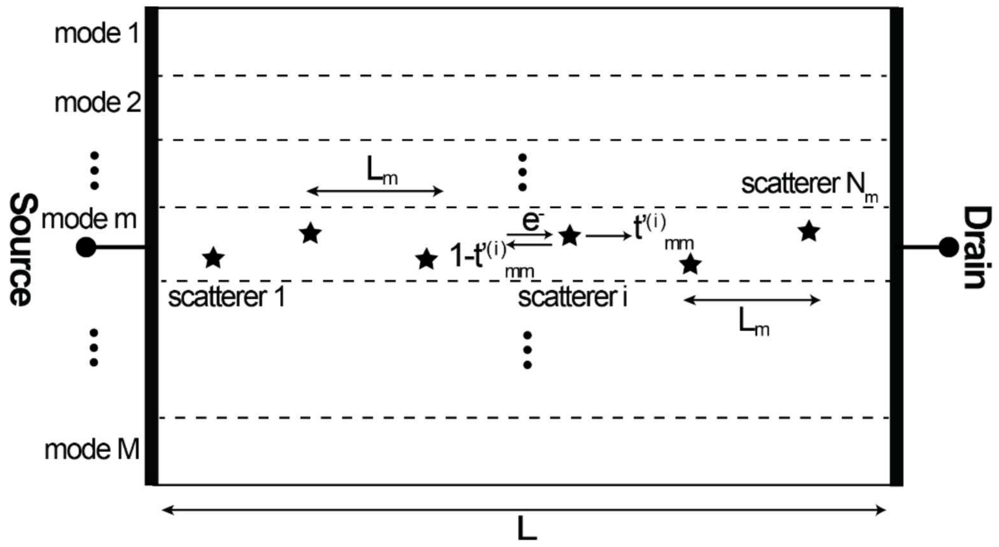




- Sharp doping profile reduces the current leakage

$N_D=1.2\times10^{14}\ cm^{-2}$, $N_A=10^{17}\ cm^{-3}$, W=40nm

Elastic scattering model



$T_{mm}(E) \equiv$ Electronic transmission for mode m without scatterers

$t_{mm}^{(i)}(E) \equiv$ Defect transmission probability due to scatterer i in mode m

$L_m \equiv$ mean free path

- **Effective electronic transmission**

$$T_{mm}^{\text{eff}}(E) = \frac{1}{\underbrace{1}_{\text{Contact scattering}} + \underbrace{\frac{1-T_{mm}(E)}{T_{mm}(E)}}_{\text{Geometry scattering}} + \underbrace{L\nu_m \frac{1-t'_{mm}(E)}{t'_{mm}(E)}}_{\text{Defect scattering}}}$$

$$L\nu_m \frac{1-t'_{mm}}{t'_{mm}} \equiv \mathcal{O}\left(\frac{L}{L_m}\right) \equiv \boldsymbol{\alpha} \frac{L}{L_m}$$

The parameter $\boldsymbol{\alpha}$ is proportional to the linear impurity density

- **Current density (Landauer formula)**

$$J = \frac{2e}{h} \int \sum_{m=1}^{M} T_{mm}^{eff}(E)\big(f_S(E) - f_D(E)\big)dE$$

Proof that the Quantum Simulation works!

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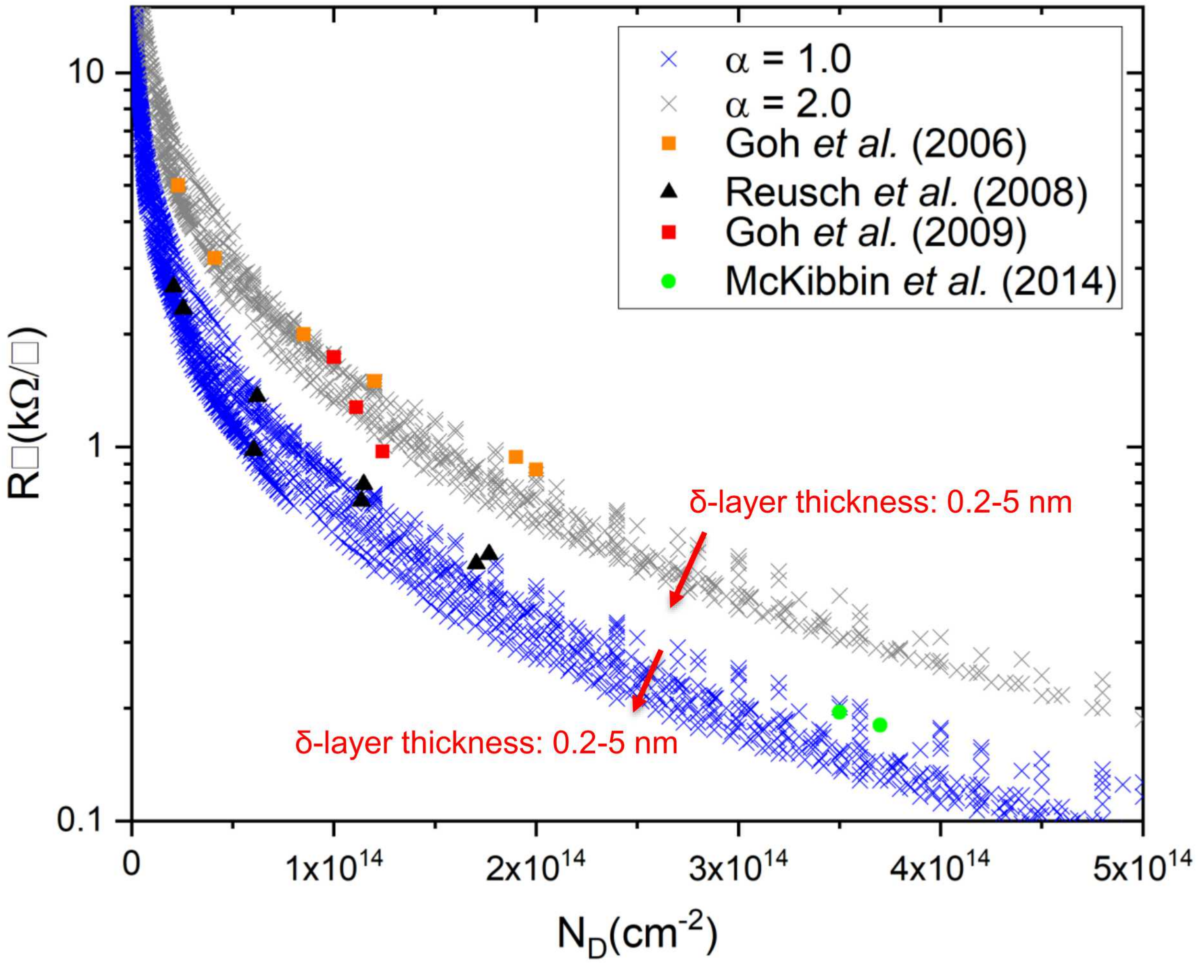
- **Our simulations accurately reproduce the experimental sheet resistances at 4 K**



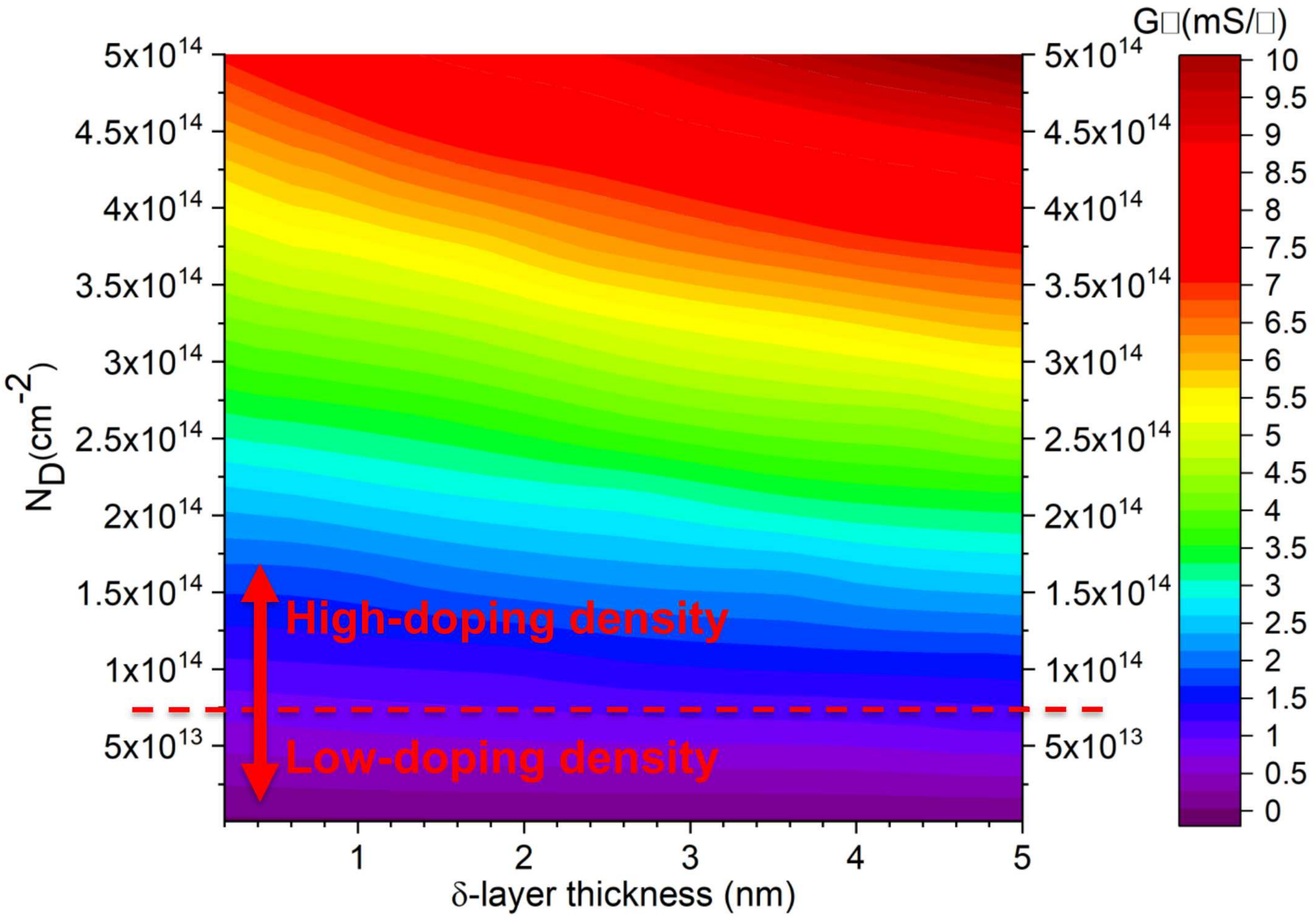
$$T^{\mathrm{eff}}_{mm}(E) = \frac{1}{1 + \frac{1 - T_{mm}(E)}{T_{mm}(E)} + \boldsymbol{\alpha} \frac{L}{L_m(N_D)}}$$

The parameter ***α*** *is proportional to the linear defect density in the system*

K. E. J. Goh *et al.*, Phys. Rev. B, vol. 73, p. 035401, 2006
K. E. J. Goh and M. Y. Simmons, Appl. Phys. Lett., vol. 95, no. 14, p. 142104, 2009
S. R. McKibbin *et al.*, Appl. Phys. Lett., vol. 104, no. 12, p. 123502, 2014
T. C. G. Reusch *et al.*, J. Appl. Phys., vol. 104, no. 6, p. 066104, 2008

Sheet conductance for Si: P δ-layer wires

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



Summary

- Presented a fully quantum **open-system transport simulations** for Si: P δ-layer systems, including a **elastic scattering model**

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

- Predicted **quantum thickness dependence** on the conductive properties

- Excellent agreement with experimental sheet resistance data


thank you
danke
рахмат
謝謝
ngiyabonga
teşekkür ederim
Баярлалаа
спасибо
faafetai lava
mersi
kia ora
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vinaka
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blagodaram
dank je
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maururu
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