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Quantum Transport Simulations for Si: P δ-layer Tunnel Junctions

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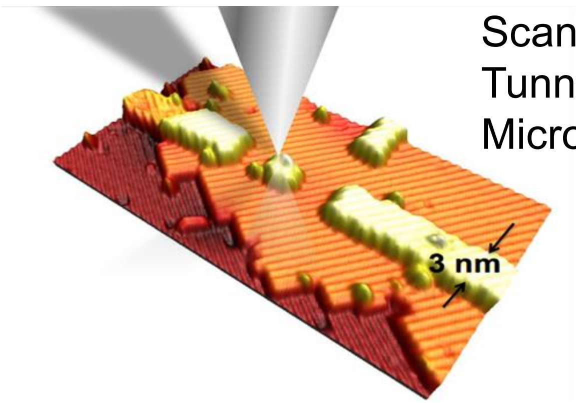
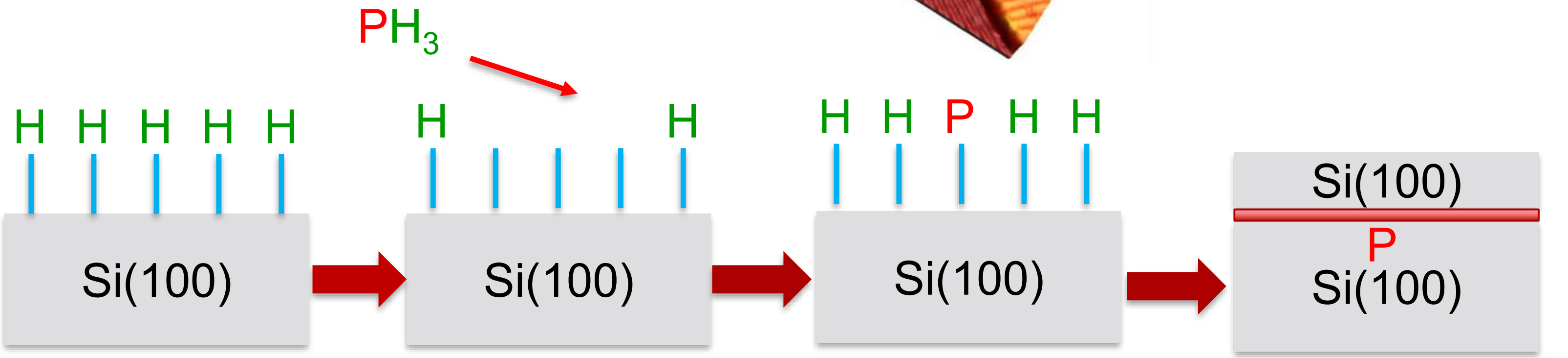
Motivation

Atomic Precision Advanced Manufacturing (APAM)

is a process of area-selective dopant incorporation at the atomic scale



STM = Scanning Tunneling Microscope



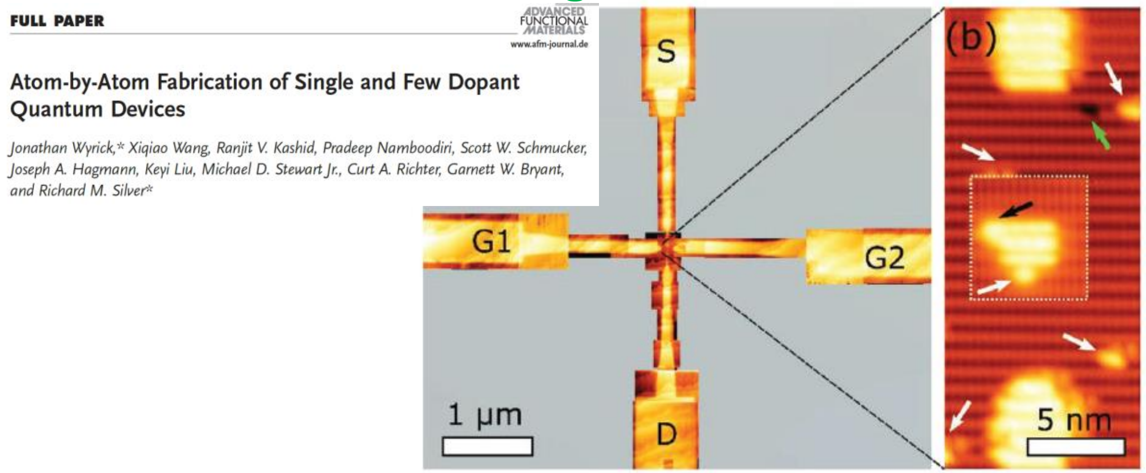
H-terminated surface

STM patterning with PH_3 precursor

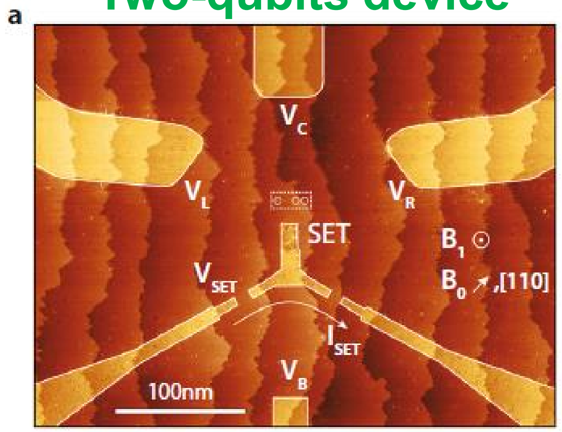
P incorporation at atomic scale

Locking layer & Encapsulation

Single atom transistor

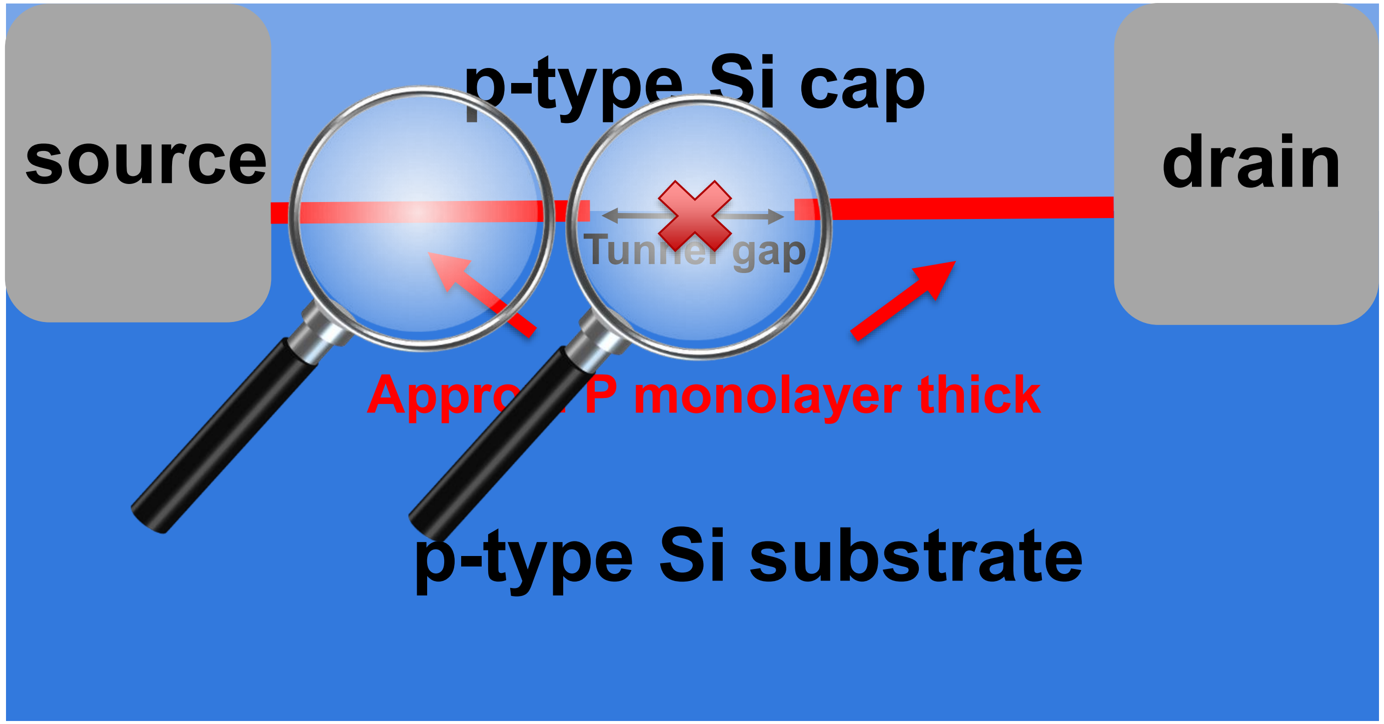


Two-qubits device



Si: P delta-layer Tunnel Junction

- High potential for **quantum computing** and **advanced microelectronic devices**



Open-system Quantum Transport Framework

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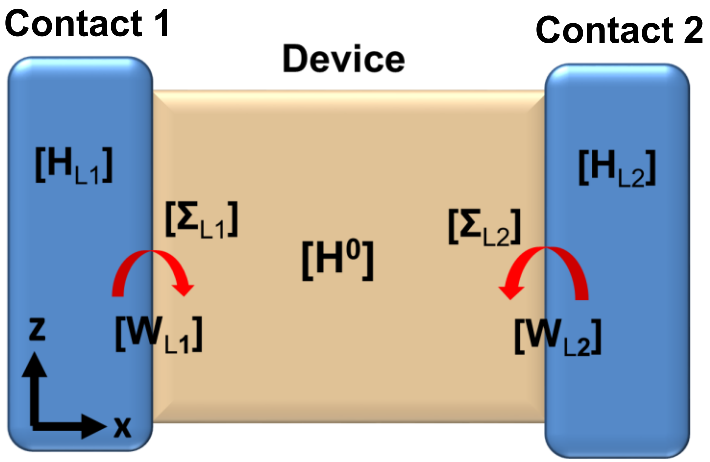
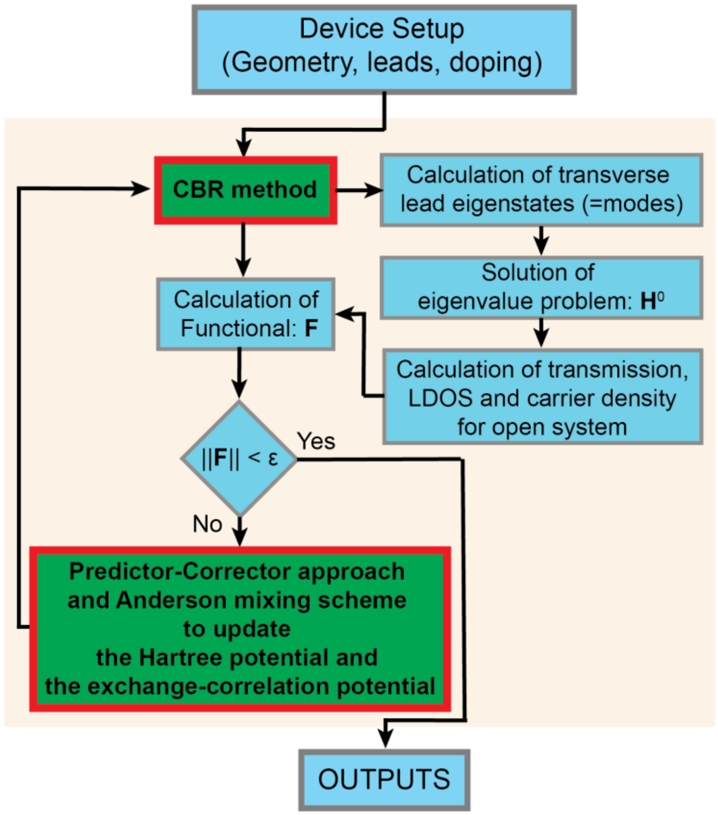
Our quantum transport simulator is based on **Non-Equilibrium Green's function** (NEGF) formalism with

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



Quantum transport simulator



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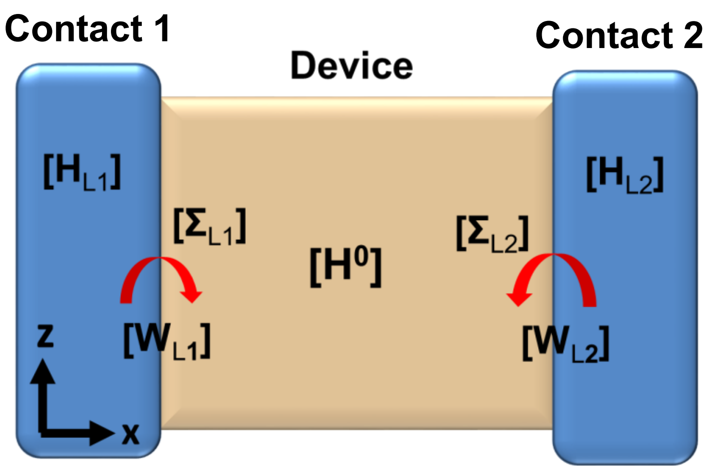
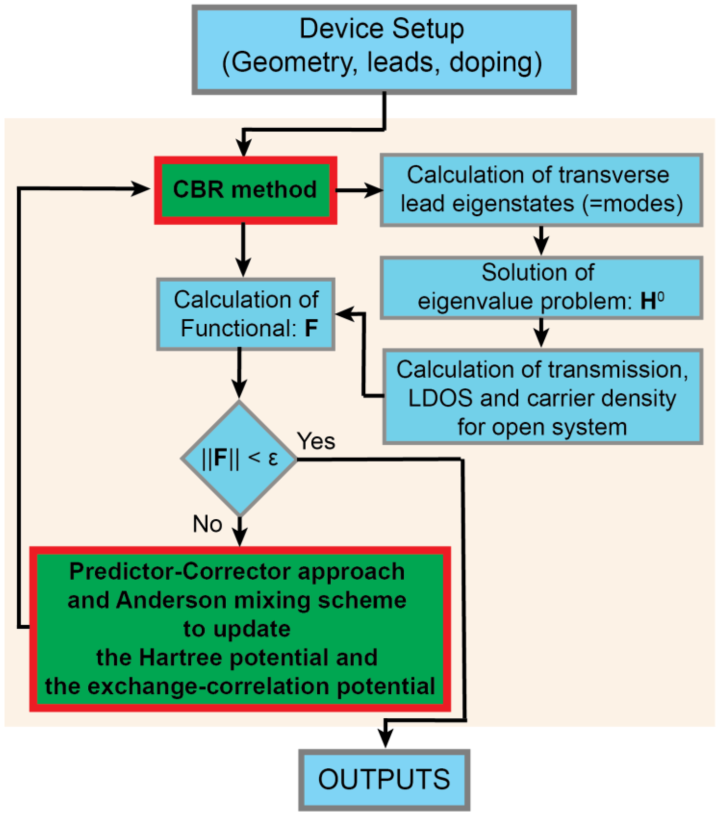
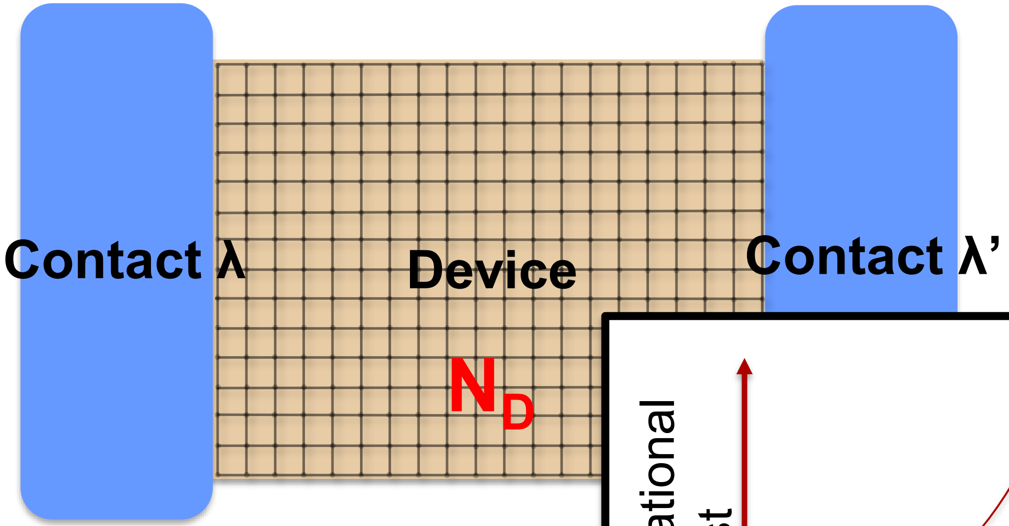


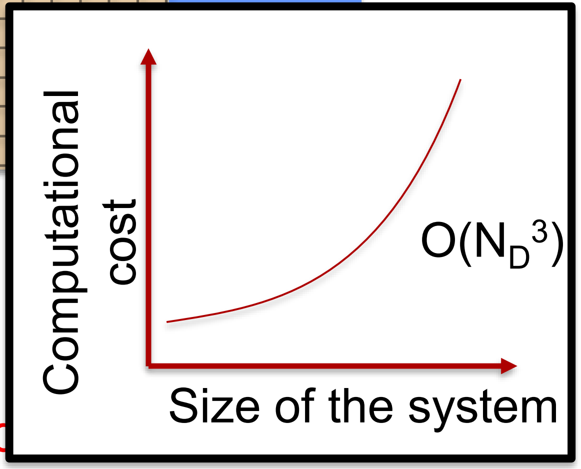
Quantum transport simulator



- 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'**

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

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

Self-energy matrix of lead

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

Open-device Hamiltonian matrix

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

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

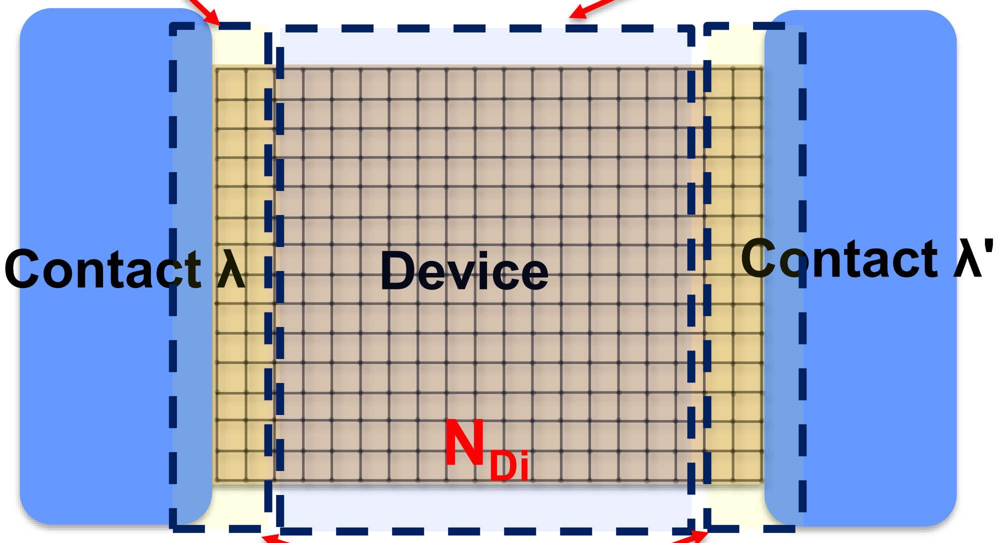
$(N_D \times N_D)$

- **Electron density**

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

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

Contact Block Reduction Method



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

$$H_D = \begin{pmatrix} H_C & H_{CD_i} \\ H_{D_iC} & H_{D_i} \end{pmatrix}$$

$(N_D \times N_D)$; H_C: $(N_C \times N_C)$; H_{CD_i}: $(N_C \times N_{Di})$; H_{D_i}: $(N_{Di} \times N_{Di})$

$$G_D = \begin{pmatrix} G_C & G_{CD_i} \\ G_{D_iC} & G_{D_i} \end{pmatrix}$$

$$\Sigma = \sum_{\lambda=\lambda_1}^{\lambda_L} \Sigma_\lambda = \begin{pmatrix} \Sigma_C & 0 \\ 0 & 0 \end{pmatrix}$$

- **Electrical current:**

$$J_{\lambda\lambda'} = \frac{2e}{h}\int T_{\lambda\lambda'}(E)(f_\lambda(E) - f_{\lambda'}(E))dE, \quad T_{\lambda\lambda'}(E) = \mathrm{Tr}(\Gamma_{C_\lambda} G_C \Gamma_{C_{\lambda'}} G_C^\dagger), \quad G_C = [I - G_C^0 \Sigma_C]^{-1} G_C^0$$

- **Electron density:**

$$\rho(r_i) = \int_{-\infty}^{\infty} \Xi(E) f_\lambda(E) dE, \quad \Xi(E) = \frac{1}{2\pi}\frac{\mathrm{Tr}[B_C^{-1}\Gamma_C B_C^{-1\dagger}]}{(E^+ - E_\alpha)(E^- - E_\alpha)}, \quad B_C = 1_C - \Sigma_C G_C^0$$

$(N_C \times N_C)$

Last year in SISPAD 2020 …

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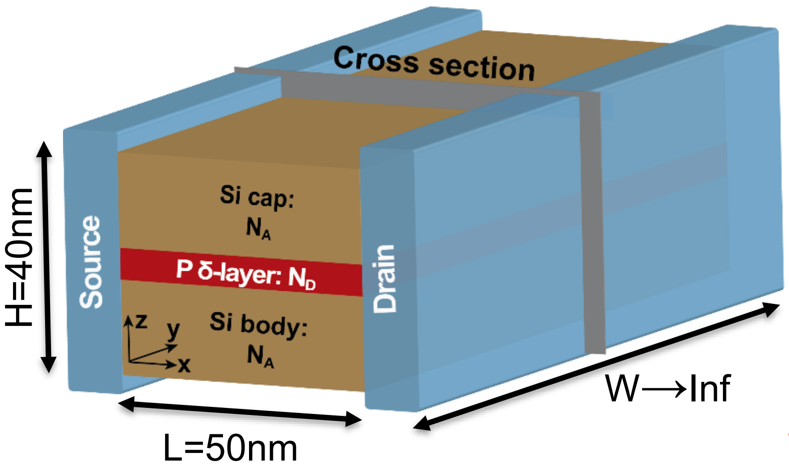
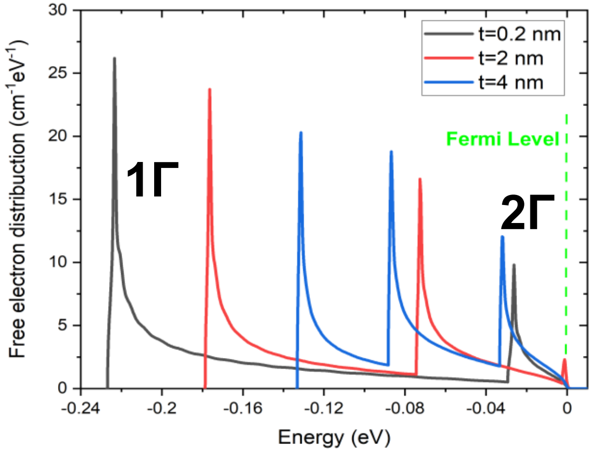
Infinite-width δ-layer systems:

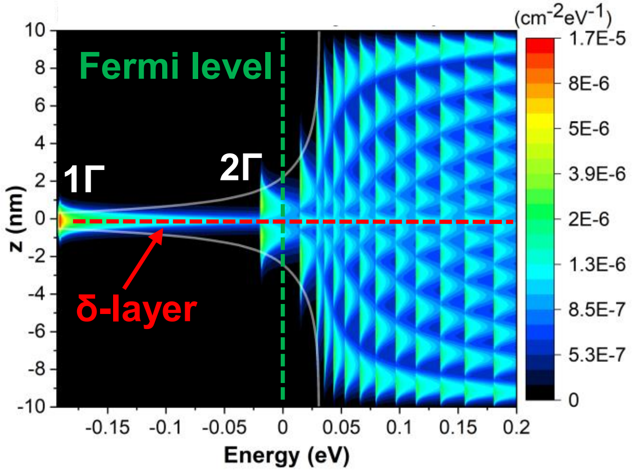


$N_D=1.2\times10^{14}$ cm^{-2}, $N_A=10^{17}$ cm^{-3}

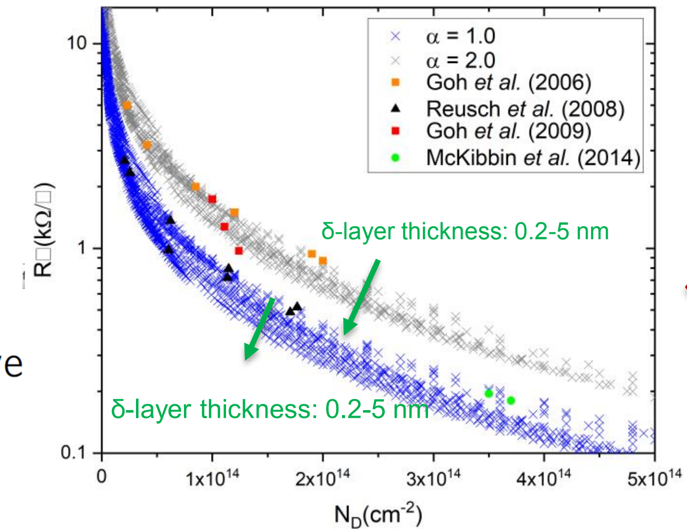
- **Prediction of shallow Sub-bands**



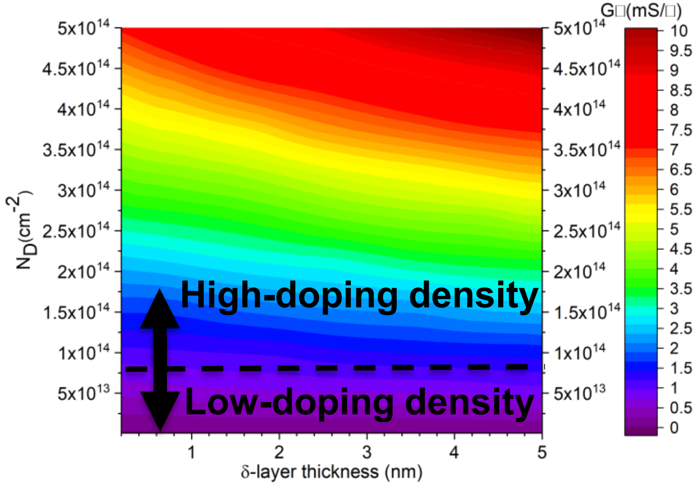
- **The so-called "quantum menorah": LDOS(E,z)**



- **Good agreement with experiments at 4K!!**



- **Quantum thickness dependence on the sheet conductance**



communications physics

ARTICLE

https://doi.org/10.1038/s42005-021-00705-1 OPEN

Revealing quantum effects in highly conductive δ-layer systems

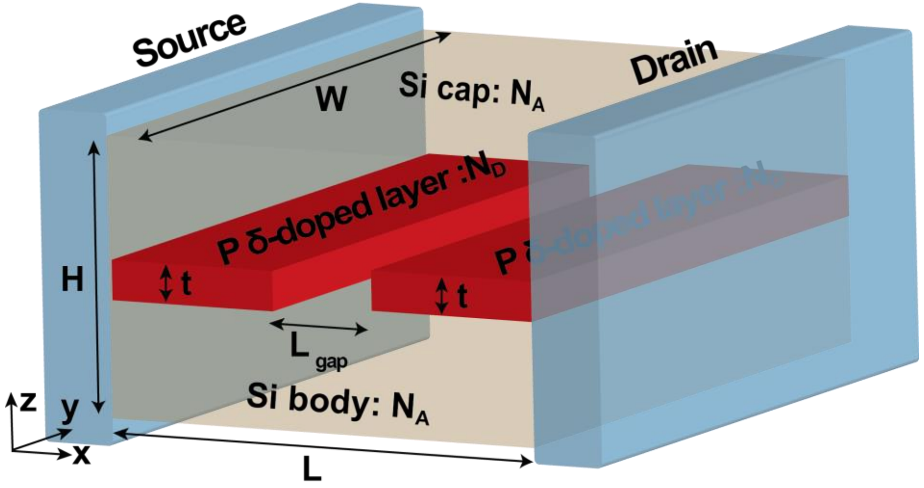
Denis Mamaluy[1], Juan P. Mendez[1], Xujiao Gao[1] & Shashank Misra[1]

https://www.nature.com/articles/s42005-021-00705-1

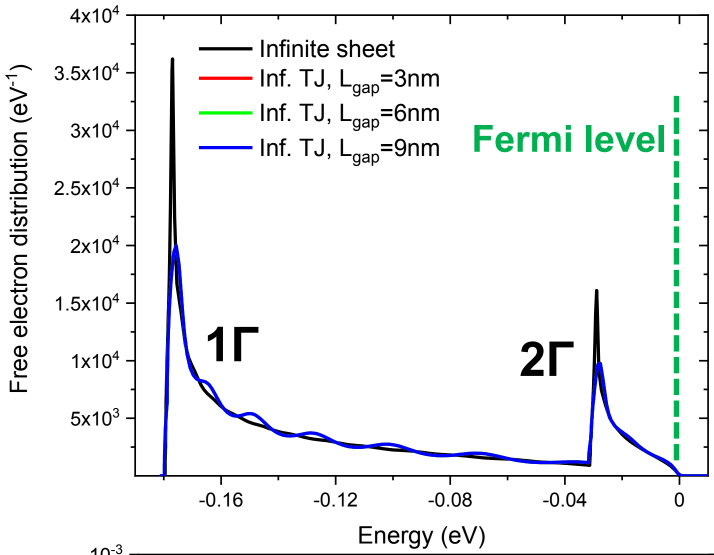
Conductive Properties for Ideal Tunnel Junctions

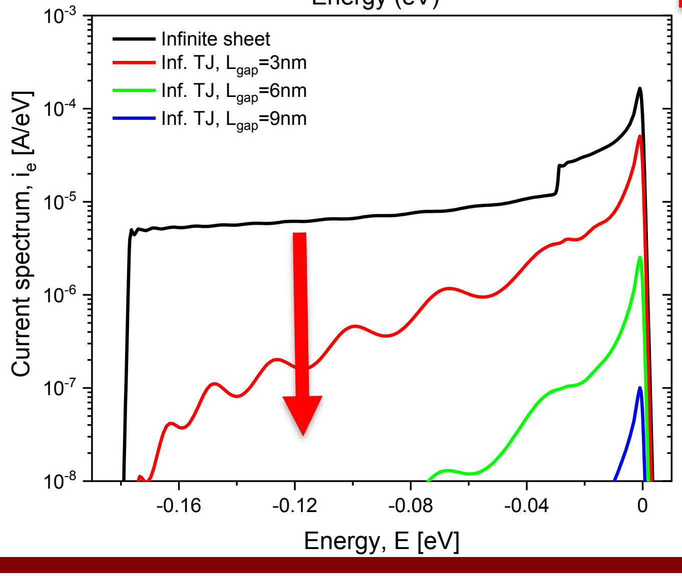
- **Low-energy electrons contribution on the current is depressed with the tunnel gap**

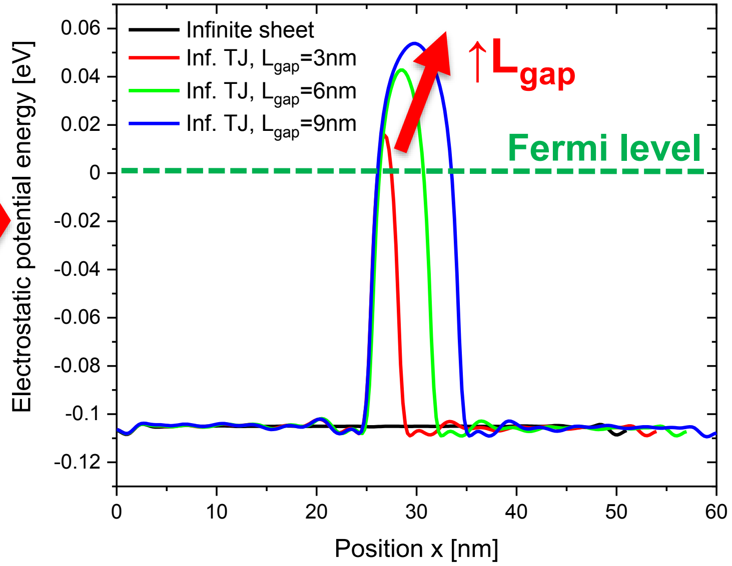
Infinite-width δ-layer Tunnel Junctions



t=1nm, N_D=1.0×10^{14} cm^{-2}, N_A=10^{17} cm^{-3}

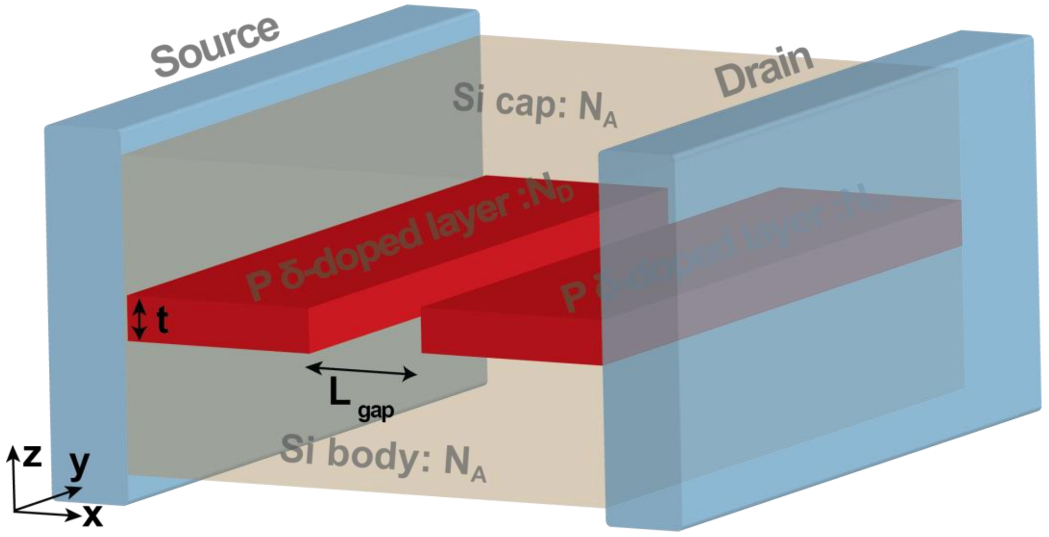




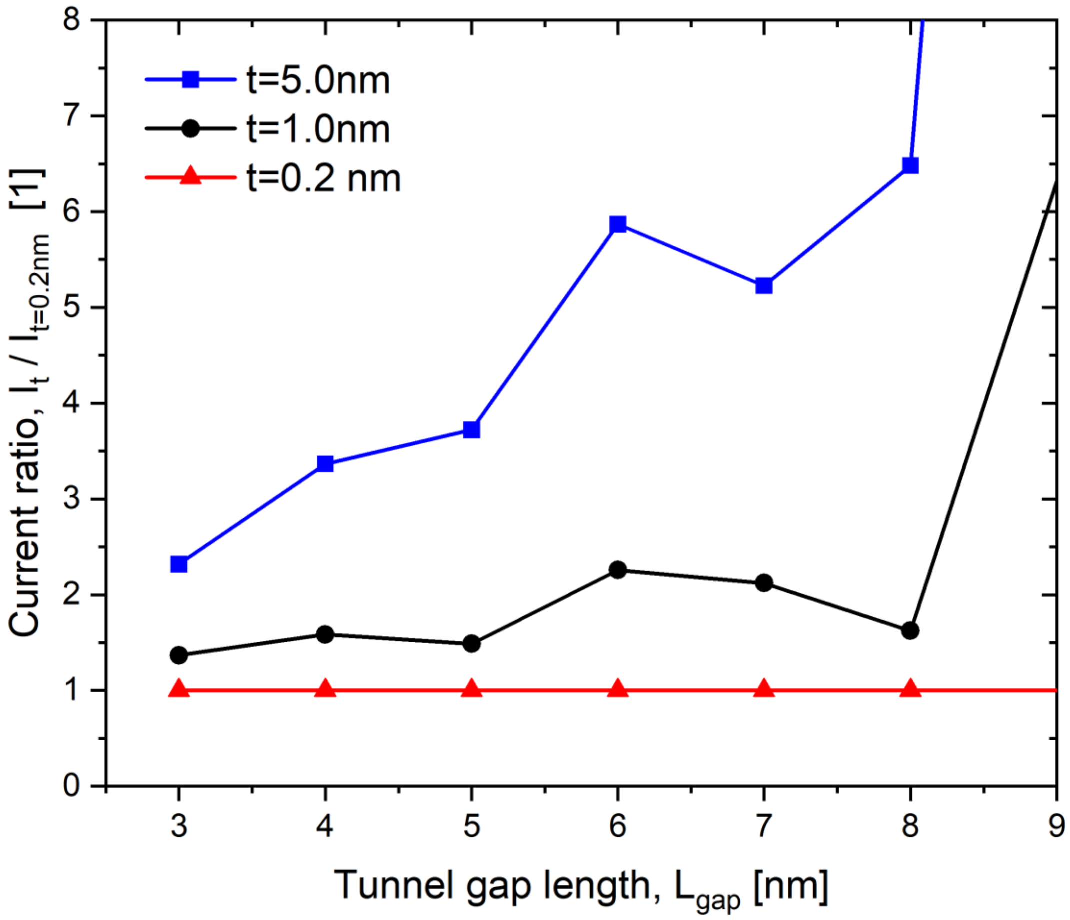


Variation of the δ-layer thickness

- **The tunneling rate considerably increases with the δ-layer thickness, specially for larger tunnel gaps**

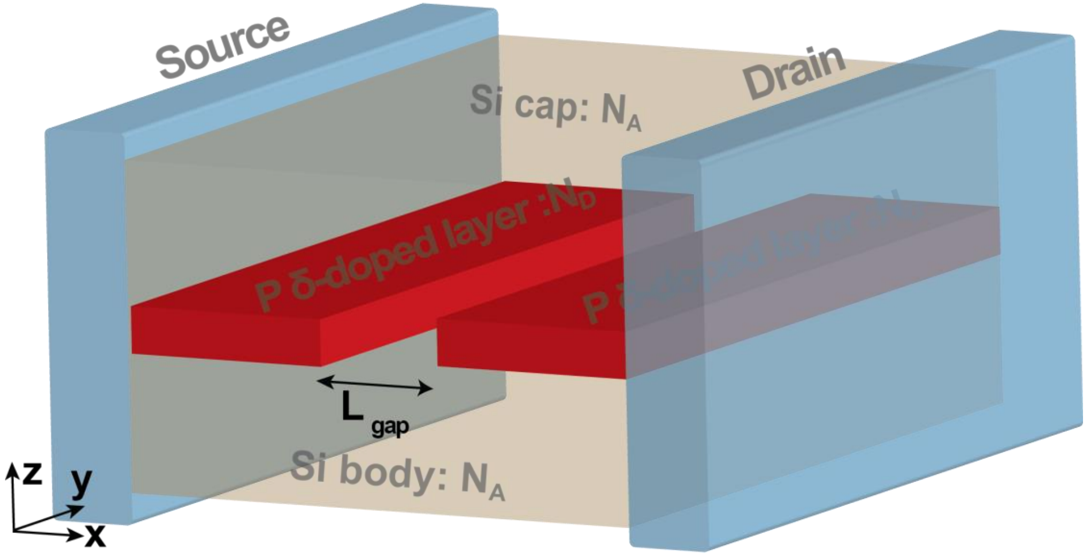


N_D=1.0×10^{14} cm^{-2}, N_A=10^{17} cm^{-3}

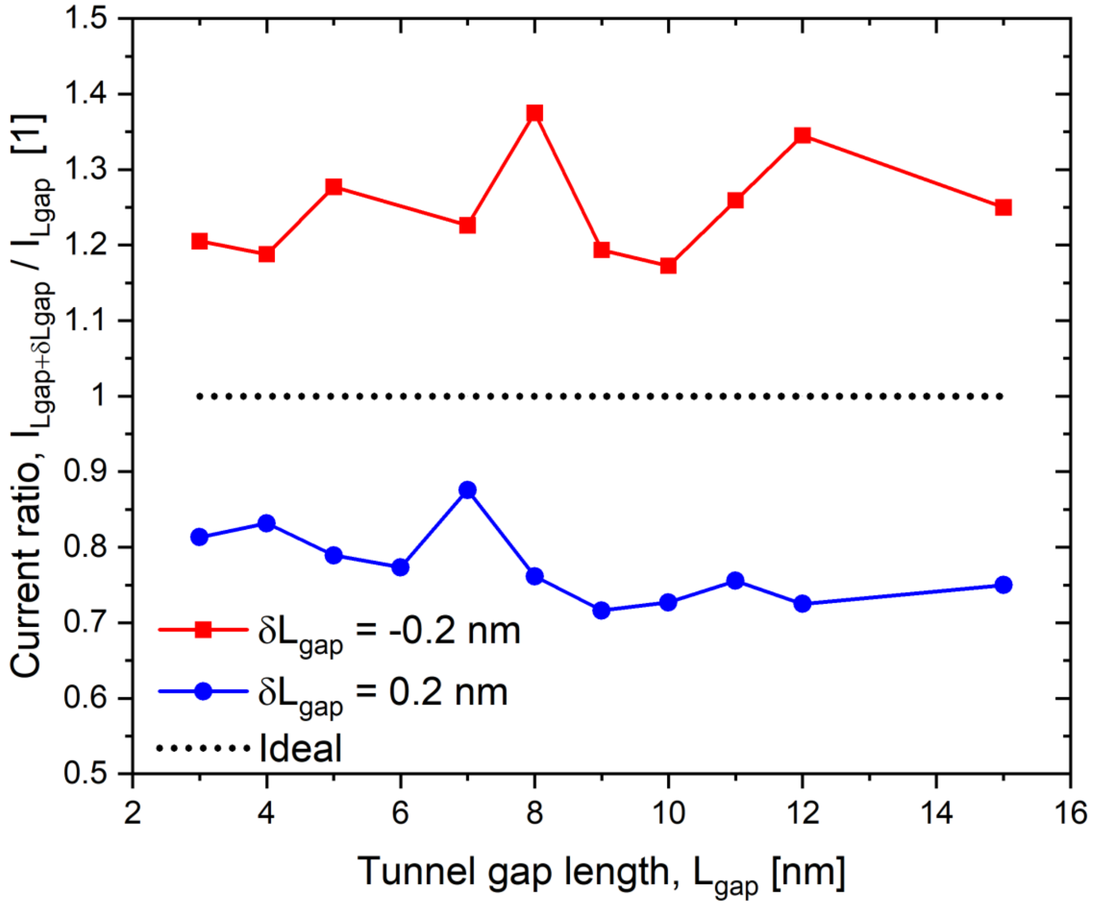


Variation of the tunnel gap length

- **Small variations of the gap length (around 0.2 nm) leads to a tunneling rate change of around 20%-30%**

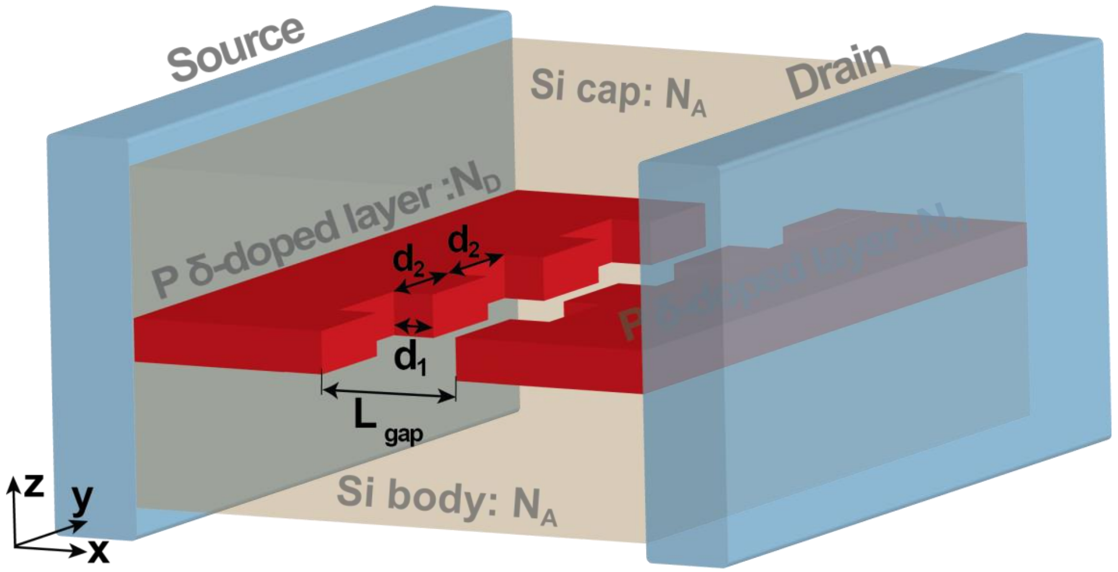


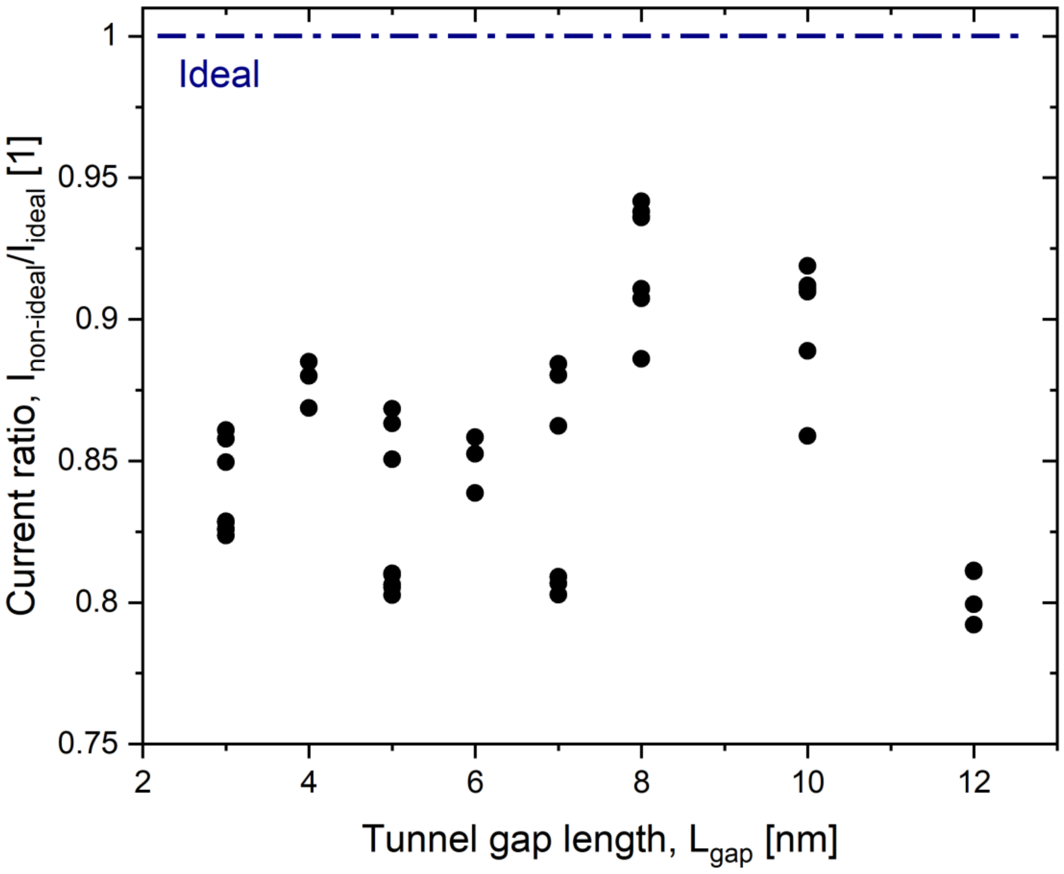
N_D=1.0×10^{14} cm^{-2}, N_A=10^{17} cm^{-3}



Effects of Edge roughness

- **Edge roughness might lead to a decreases of the tunneling rate up to 5%-25%**



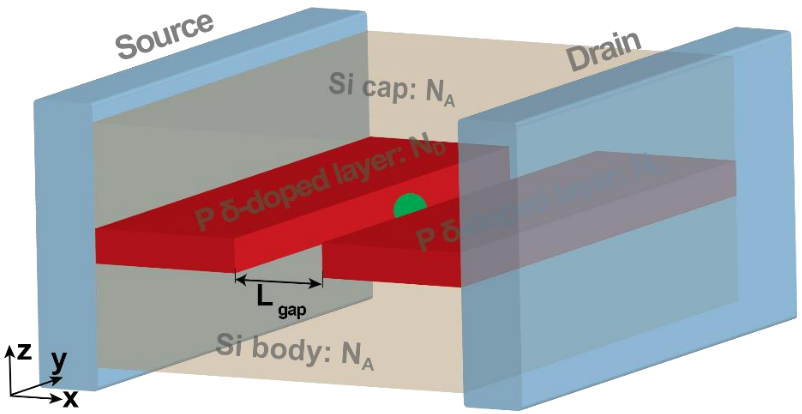


N_D=1.0×10^{14} cm^{-2}, N_A=10^{17} cm^{-3}

d_1= 0.8-2.0 nm and d_2=0.6-3.4 nm

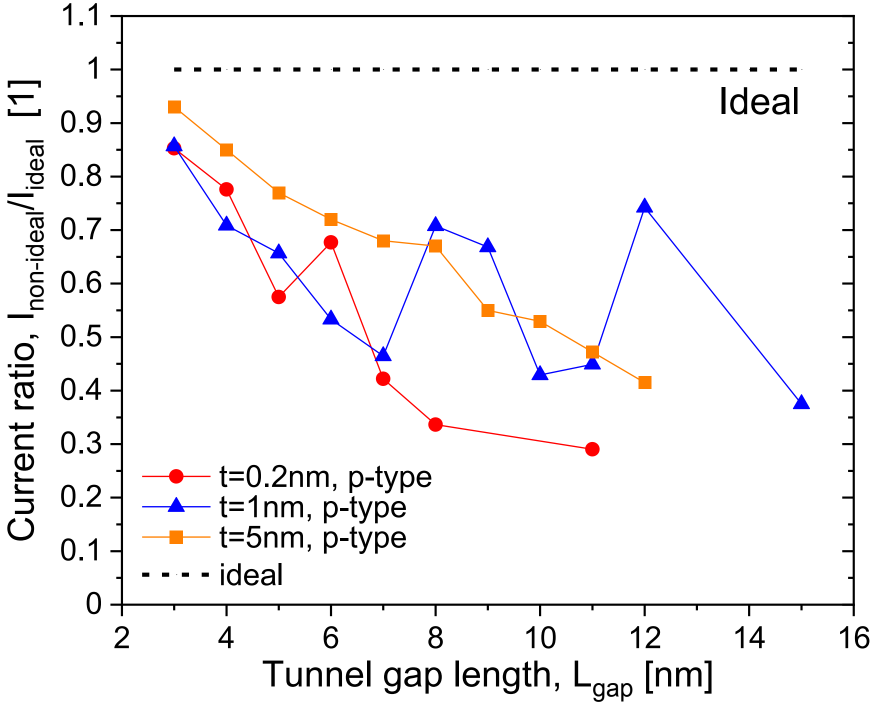
Effects of a Single Impurity in the Tunnel Gap

- **While p-type impurities might moderately reduce the tunneling rate, n-type impurities might dramatically increase the tunneling rate, specially for tunnel gaps of the order of 10 nm**

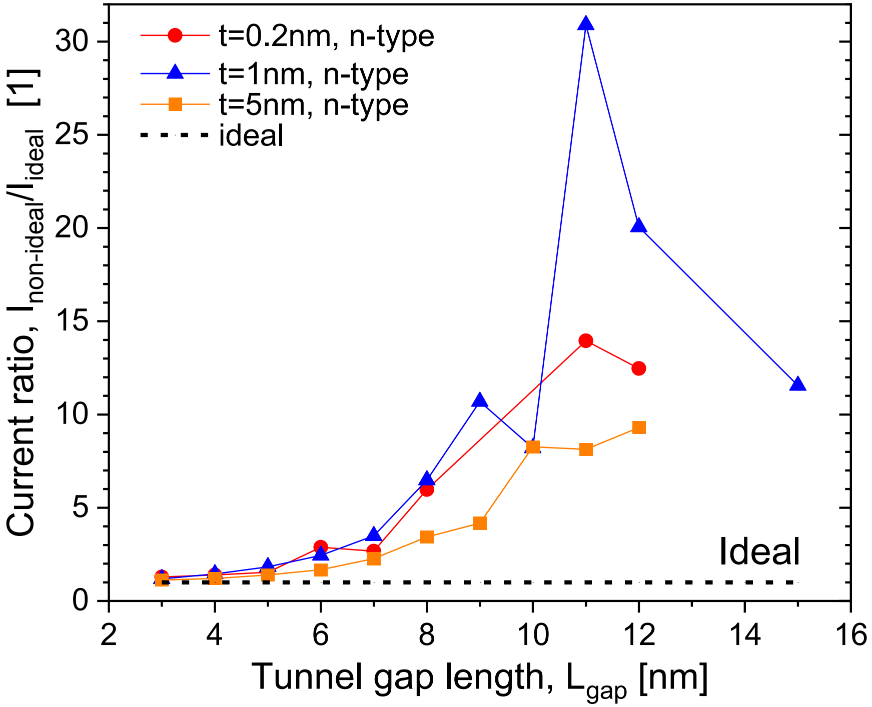


N_D=1.0×10^{14} cm^{-2}, N_A=10^{17} cm^{-3}

p-type impurity



n-type impurity



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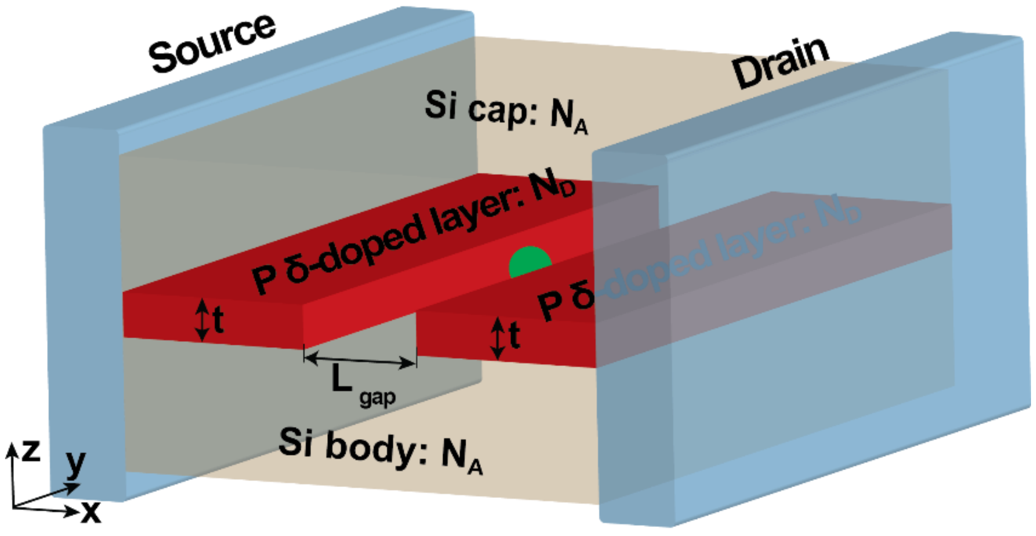

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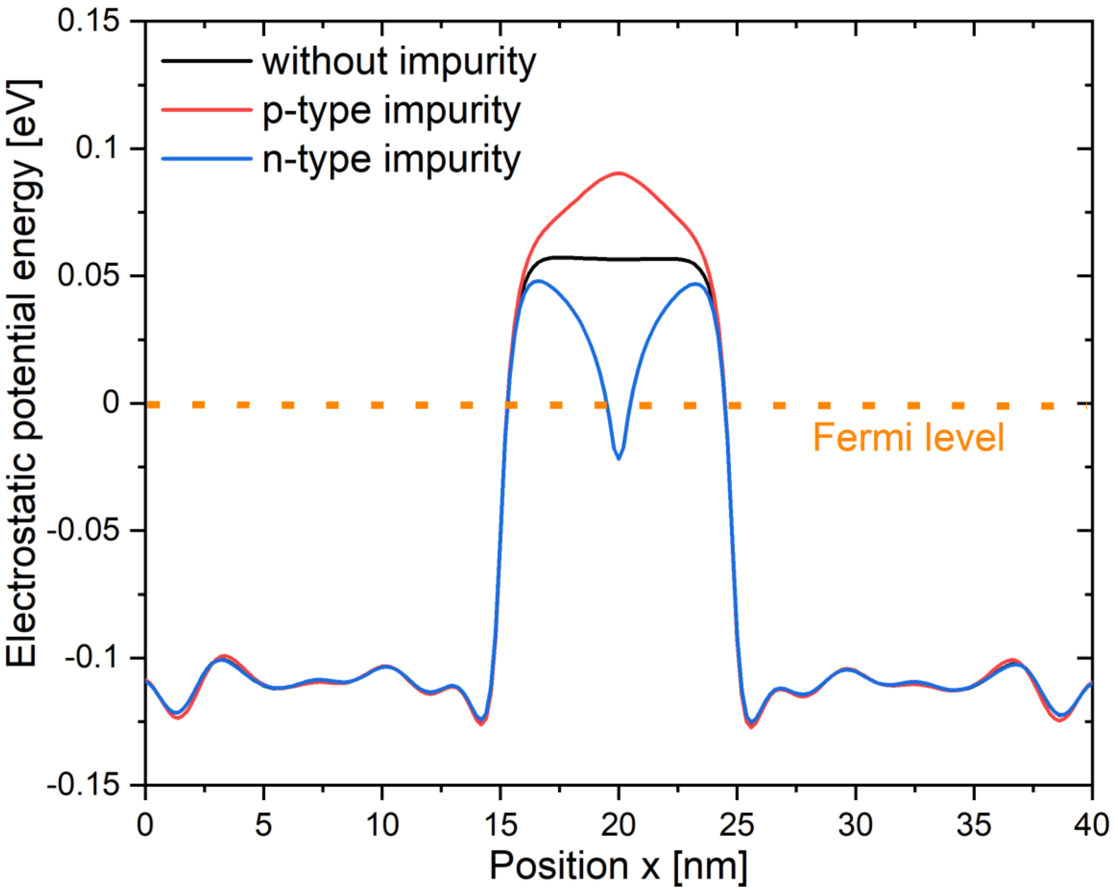

Summary

- Presented an **efficient quantum open-system transport framework** for δ-layer tunnel junctions

- While most of the non-idealities moderately affect the tunneling rate, a **single charged impurity** in the tunnel gap can alter the tunneling rate by more than an **order of magnitude**, even for relatively large tunnel gaps

- The electric **sign of impurity** plays an important role in the tunneling rate: the change of current due to an n-type impurity is an order of magnitude stronger than for p-type impurity

- Overall these simulations suggest that **geometric fidelity of the device fabrication is less important than mitigation of defects inside of the junction**


thank you
рахмат
danke
謝謝
ngiyabonga
teşekkür ederim
Баярлалаа
спасибо
faafetai lava
mersi
kia ora
barka
welalin
tack
spas
dank je
misaotra
matondo
paldies
grazzi
mahalo
tapadh leat
vinaka
спасибі
blagodaram
kiitos
dankie
gracias
хвала
nanni
nandri
dhanyavad
maururu
köszönöm
asante
manana
obrigada
tenki
bedankt
bayarlalaa
gràcie
hvala
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djiere dieuf
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murakoze
enkosi
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