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Prediction of two conductivity regimes in δ-layer tunnel junctions

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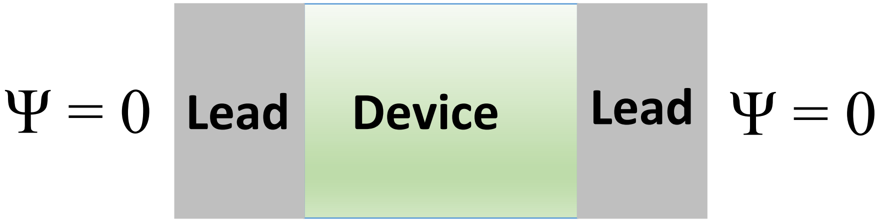
Open system approach to band structure calculation

Traditional methods

Closed system Boundary Conditions



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

$$J = en\mu E \sim |\Psi|^2$$

**This approximation is not valid for δ-layer systems.

VS

Our approach

Open system Boundary Conditions

→Extract the conductive properties from the quantum flux**

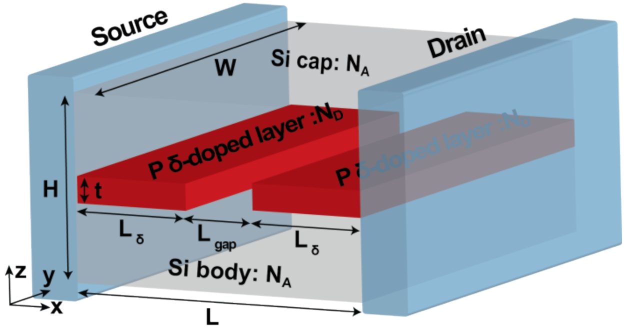
$$J \sim \Psi \nabla \Psi^* - \Psi^* \nabla \Psi$$

**The exact quantum-mechanical result.

- Our Quantum Transport simulator (CBR code) is based on the **Open-system** Non-Equilibrium Green Function Formalism. In this work we propose to use the effective mass Hamiltonians to describe the electron transport in Si:p-type δ-layer (e.g. Si: P δ-layer) systems by solving fully charge self-consistently the appropriate open-system Schrodinger-Poisson equations.
- The open-system treatment will allow to compute the conducting properties of Si:P δ-layer systems from ***first quantum-mechanical principles***, avoiding approximations intrinsic to the traditional (closed-system) band-structure methods.

Revealing quantum effects in n highly conductive δ-layer systems https://www.nature.com/articles/s42005-021-00705-1

Experimental confirmations



communications physics

ARTICLE

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

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Revealing quantum effects in highly conductive δ-layer systems

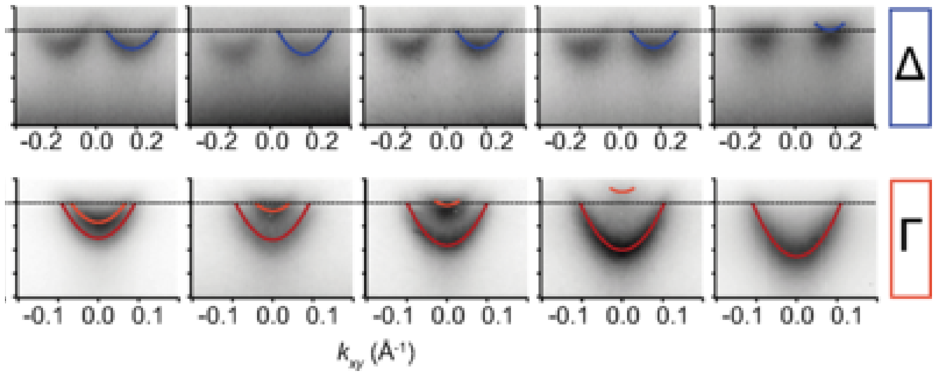
Denis Mamaluy[1✉], Juan P. Mendez[1✉], Xujiao Gao[1] & Shashank Misra[1]

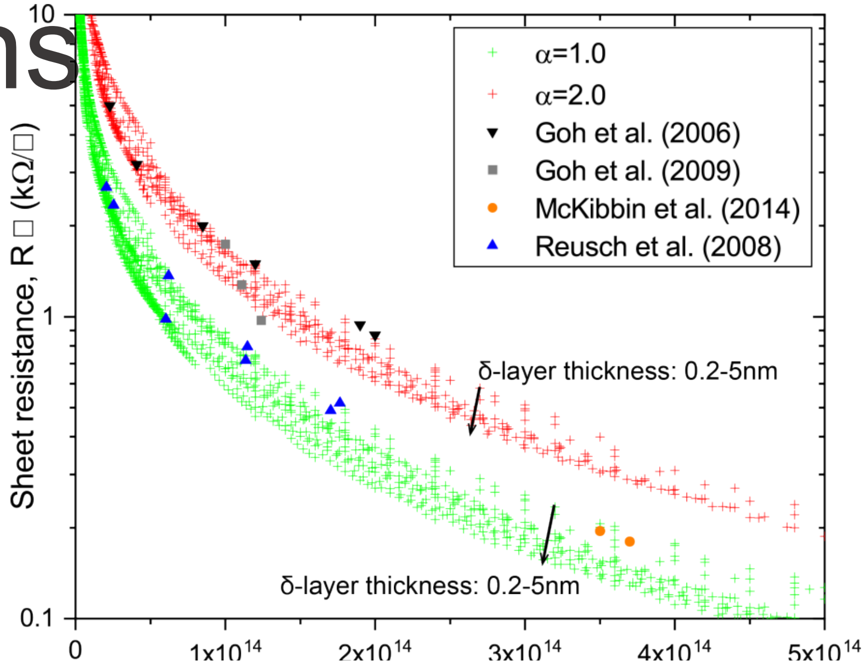
PHYSICAL REVIEW B **101**, 121402(R) (2020)

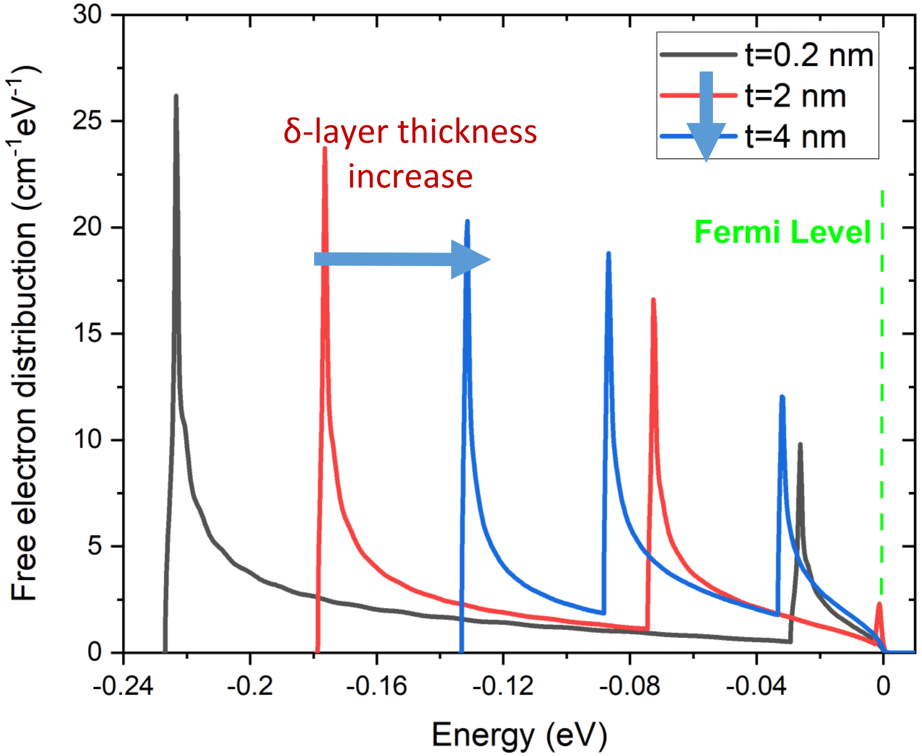
Rapid Communications

Observation and origin of the Δ manifold in Si:P δ layers

Ann Julie Holt,[1] Sanjoy K. Mahatha,[1] Raluca-Maria Stan,[1] Frode S. Strand,[2] Thomas Nyborg,[2] Davide Curcio,[1] Alex K. Schenk,[2] Simon P. Cooil,[2,3] Marco Bianchi,[1] Justin W. Wells,[2] Philip Hofmann,[1] and Jill A. Miwa[1,*]







Unexplained I-V measurements in δ-layer n_{++}-n_i-n_{++} tunnel junctions

NANO LETTERS

pubs.acs.org/NanoLett

Monolithic Three-Dimensional Tuning of an Atomically Defined Silicon Tunnel Junction

Matthew B. Donnelly,* Joris G. Keizer, Yousun Chung, and Michelle Y. Simmons

Cite This: *Nano Lett.* 2021, 21, 10092–10098 Read Online

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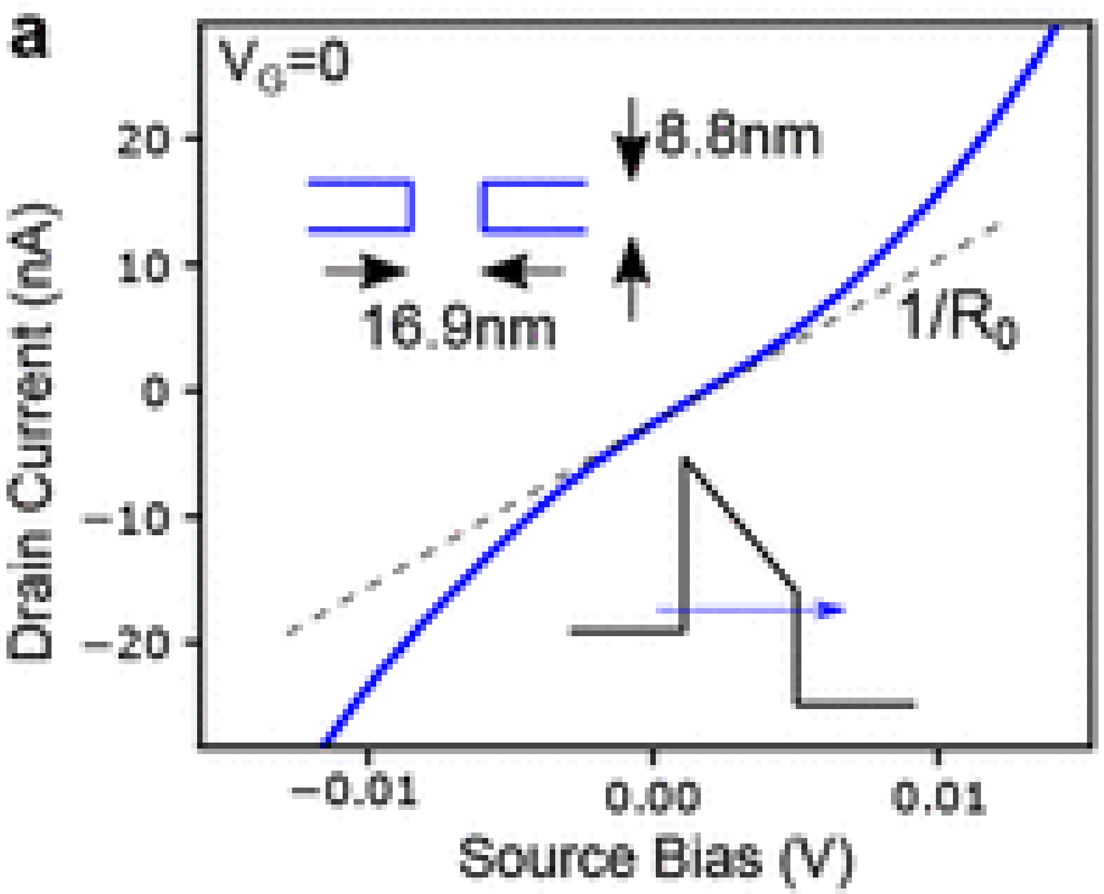

Similar "flattened" I-V characteristics were reported for delta-layer p-n junctions

nature electronics

ARTICLES

https://doi.org/10.1038/s41928-020-0445-5

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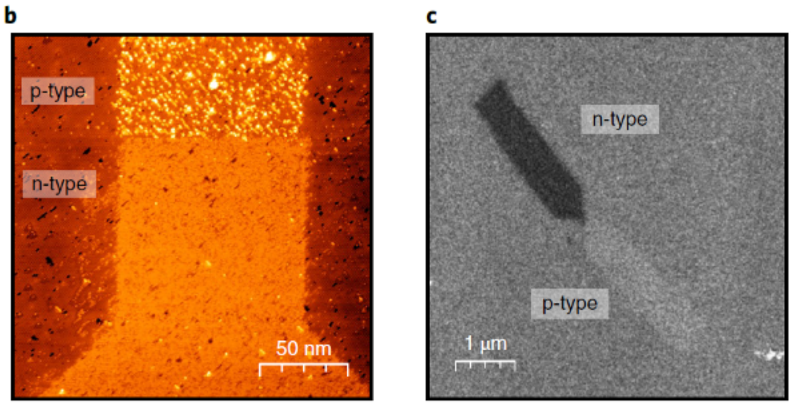
Bipolar device fabrication using a scanning tunnelling microscope

Tomáš Škereň[1], Sigrun A. Köster[1], Bastien Douhard[2], Claudia Fleischmann[2] and Andreas Fuhrer[1]

[*] Nature Electronics 3, 524–530 (2020)

STM image of the p-n junction



Characteristic I-V curves for the p-n junction

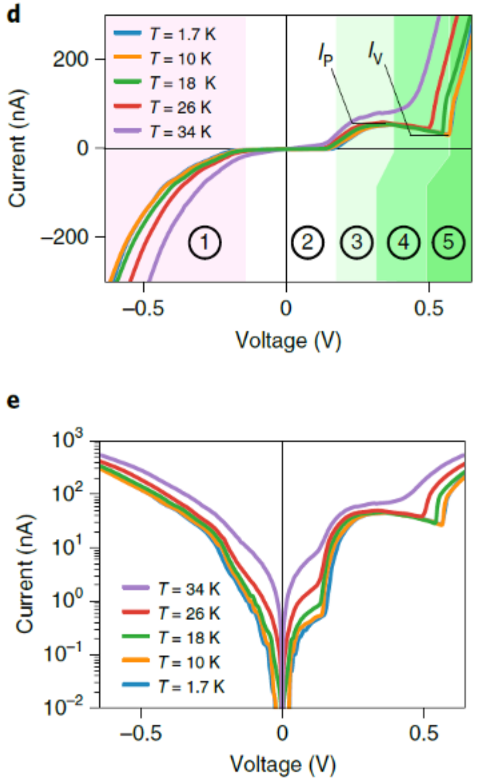


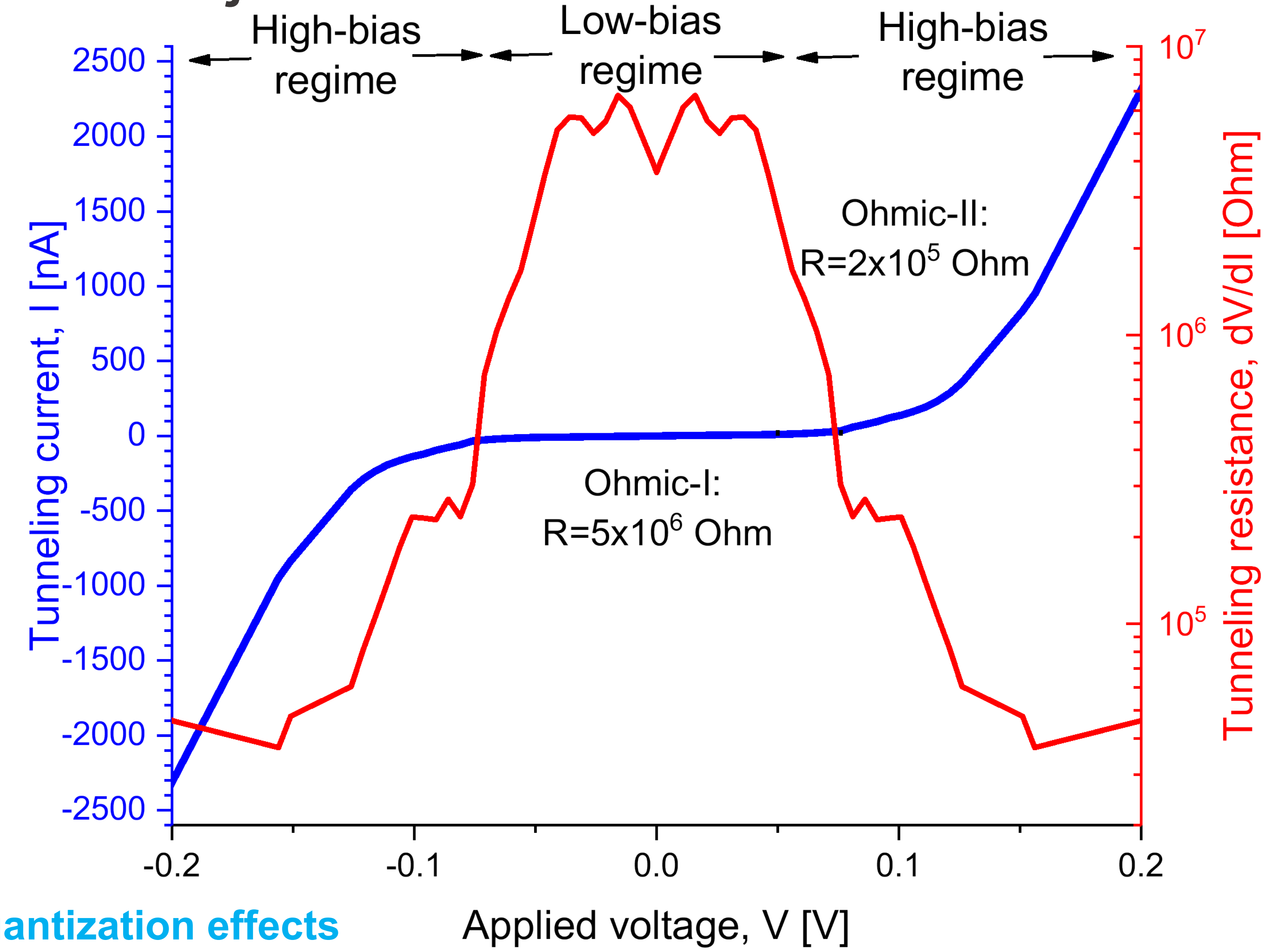
Fig. 5 | Fabrication of a bipolar dopant device with STM lithography. a, Preparation procedure. **b**, STM image of the central part of the p–n junction after desorption of the area for phosphorus doping (lower section). In the upper section, the boron-doped and incorporated area is visible. **c**, Ex situ scanning electron microscope image of the p–n device from **b**. **d**,**e**, Linear (**d**) and semilogarithmic (**e**) plot of the current–voltage characteristics of the p–n junction as a function of temperature.

In region 2, near zero applied bias voltage, the current is *strongly suppressed*, which is different from conventional highly doped p–n junctions (Esaki diodes)

→ What causes the unusual I-V trend?

Can it be due to conduction and valence <u>band quantization</u>?

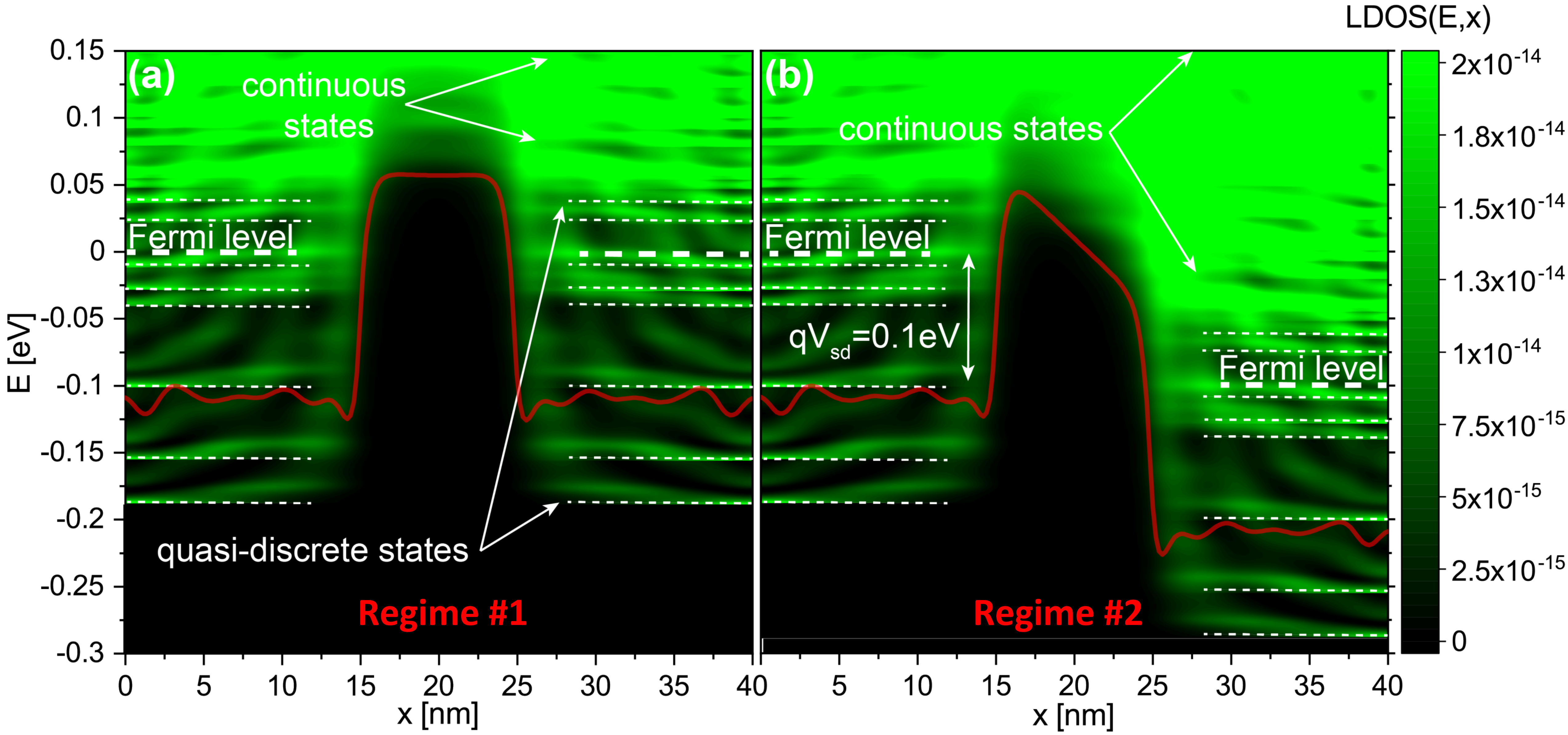
Computed (open-system) tunnel current vs voltage in delta-layer tunnel junctions



Conductivity and size quantization effects in semiconductor δ-layer systems

https://www.nature.com/articles/s41598-022-20105-x

To understand conductive properties we investigate the band structure in its real-space representation LDOS(E,r)

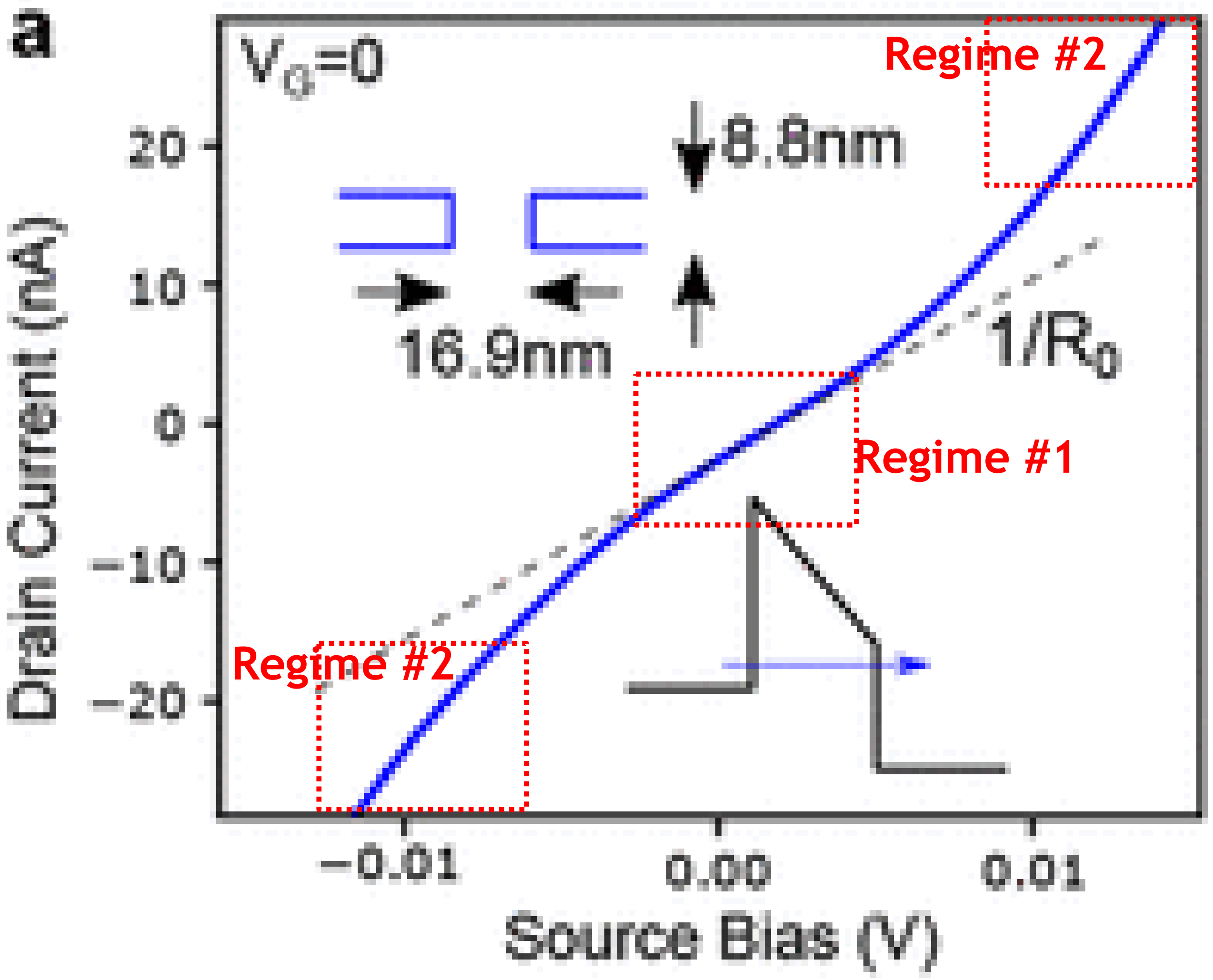


The existence of low-voltage and high-voltage regimes can be explained by the influence of band quantization effect on the conductivity.


NANO LETTERS

Monolithic Three-Dimensional Tuni
Silicon Tunnel Junction

Matthew B. Donnelly,* Joris G. Keizer, Yousun Chun



Summary

1. **Highly-confined highly-conductive** material systems and/or devices generally **require** an open-system quantum mechanical treatment (for instance – NEGF) to accurately predict the conduction band structure and the conductivity.
2. Strong **band quantization** present in nearly-monoatomic conductive delta-layers **significantly affects the conductive properties.**
3. Some of these new effects could be used in applications such as “quantum charge sensing” using δ-layers
4. There are two (**low and high voltage**) **conductivity regimes** predicted (and confirmed) in δ-layer tunnel junctions.