June 13th, 2023

δ-layer tunnel junctions in semiconductors for charge sensing

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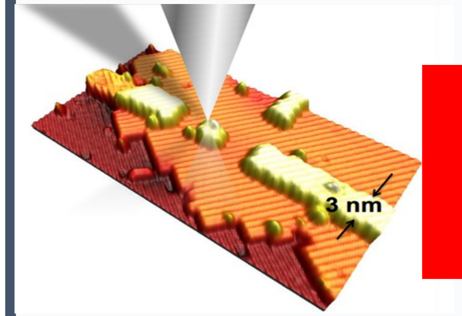
National Nuclear Security Administration

Sandia National Laboratories

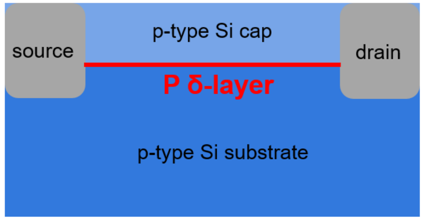
Atomic Precision Advanced Manufacturing (APAM)

APAM

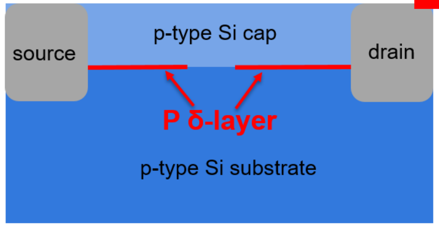


STM = Scanning Tunneling Microscope

APAM devices



Si: P δ-layer wire



Si: P δ-layer Tunnel Junction

APAM Applications

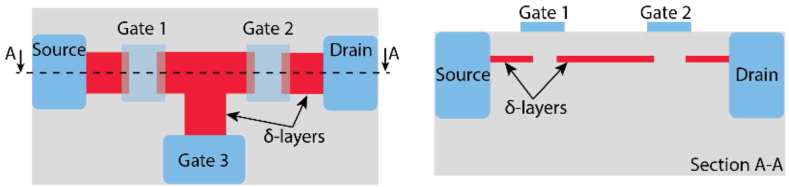
- **Beyond Moore Computing**

NANO LETTERS

pubs.acs.org/NanoLett Letter

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

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



δ-layer tunnel junction FET

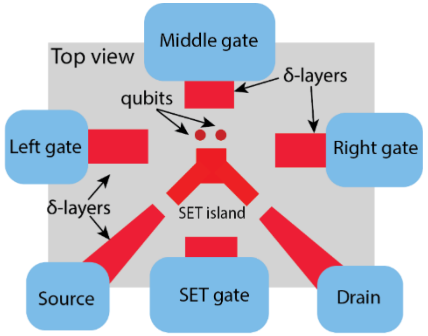
- **Quantum Computing**

LETTER

https://doi.org/10.1038/s41586-019-1381-2

A two-qubit gate between phosphorus donor electrons in silicon

Y. He[1,2], S. K. Gorman[1,2], D. Keith[1], L. Kranz[1], J. G. Keizer[1] & M. Y. Simmons[1]*



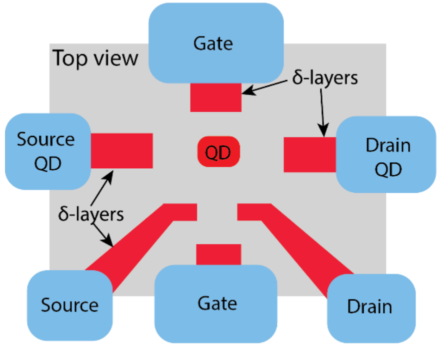
- **Novel quantum sensing**

APPLIED PHYSICS LETTERS **104**, 113111 (2014)

Single-charge detection by an atomic precision tunnel junction

M. G. House,[a)] E. Peretz, J. G. Keizer, S. J. Hile, and M. Y. Simmons[b)]

Centre for Quantum Computation and Communication Technology, University of New South Wales, Sydney, NSW 2052, Australia



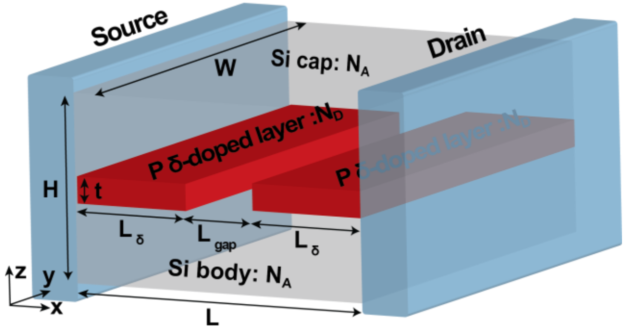
*Our computational approach for free electrons:

- Charge self-consistent NEGF implemented via Contact Block Reduction method scales linearly with the simulation volume O(V)
- Electron-electron interaction via DFT-LDA exchange-correlation
- Real-space scattering on discrete impurities
- Inelastic scattering via Matthiessen's rule and mobility models
- Kinetic energy term: the effective mass tensor

This approach allows to accurately represent all *open-system electron properties*: the current, current spectrum, transmission, LDOS.

*D. Mamaluy, J.P. Mendez *et al. Commun Phys* 4, 205 (2021)
J.P. Mendez, D. Mamaluy, *Sci Rep* 12, 16397 (2022)

Prior simulations and confirmations



communications
physics

ARTICLE

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

Check for updates

Revealing quantum effects in highly conductive δ-layer systems

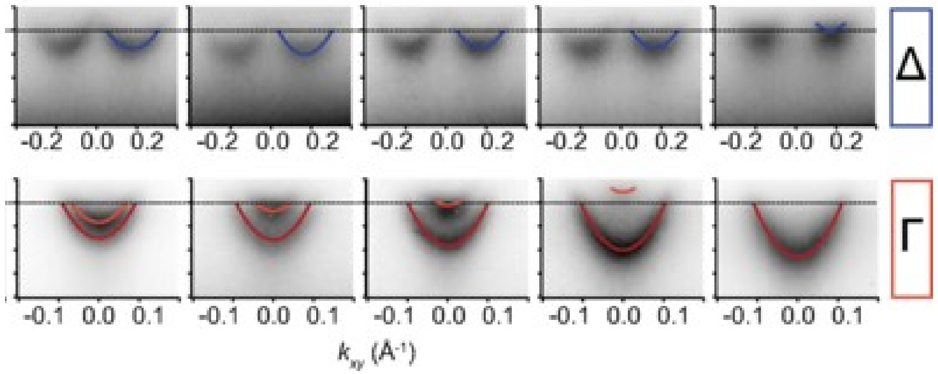
Denis Mamaluy[1✉], Juan P. Mendez[1✉], Xujiao Gao[1] & Shashank Misra[1]

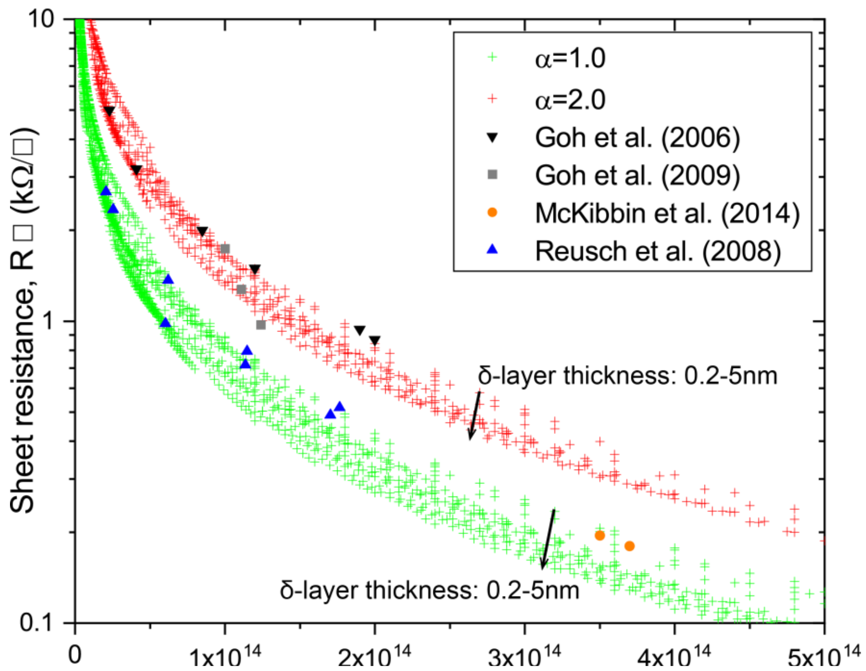
PHYSICAL REVIEW B **101**, 121402(R) (2020)

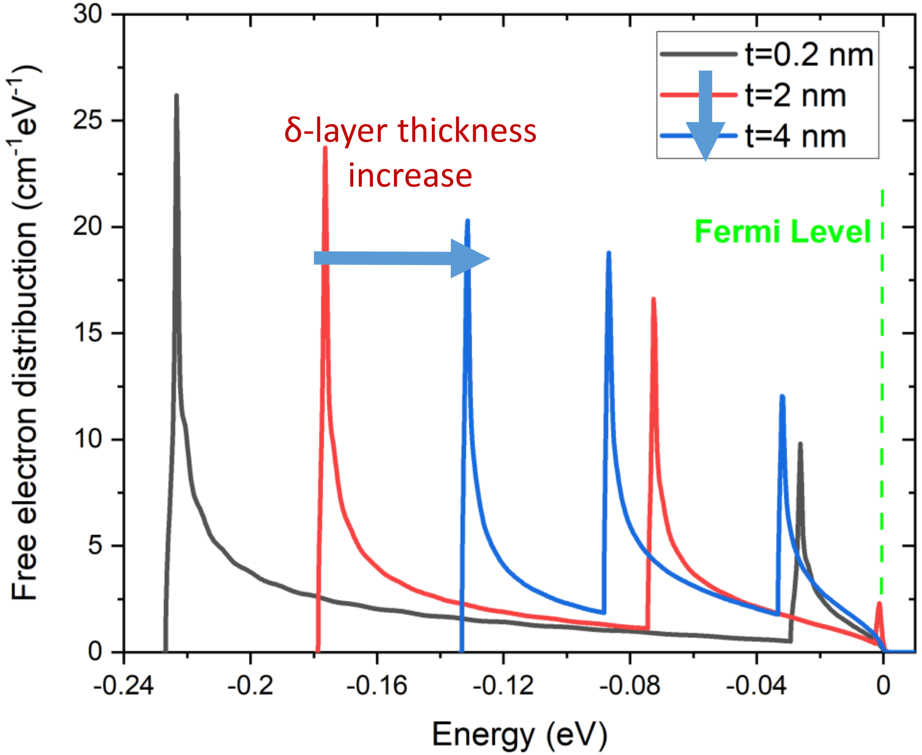
Rapid Communications

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,*]







Predictive quantum transport simulations

relaxation effects in the contacts [6].

Effective mass approaches are not predictive. At the 5nm scale a heterostructure does not only form a new device but a new composite material

composite material with new bandgaps, effective masses that cannot be predicted by bulk effective mass approaches. Atomistic basis sets are critically needed, even though transport might just happen in the conduction band. Effective mass models can be tuned to specific atomistic representations but

mod ... binding/ NEG ... 1 m_e[54,55] and ... estimates the experimental tunneling resistances. Most effective mass models are limited in terms of capturing all the band minima at different k-points. We show in Figure 2a that there are several Γ and Δ band minima at different k-points, with a notable non-parabolicity of the bands at higher k. As a result, effective mass models will tend to underestimate the density of states in the leads, leading to an overestimation of the tunneling resis ... modeling R_T is ... nge line) using ... The over- estin ... portance of us ... electronic dispersion and 3D potential profile in which excellent agreement is achieved. Our results highlight the limitations of using single-band theories such as WKB and effective mass theory to model electron tunneling transport in highly doped

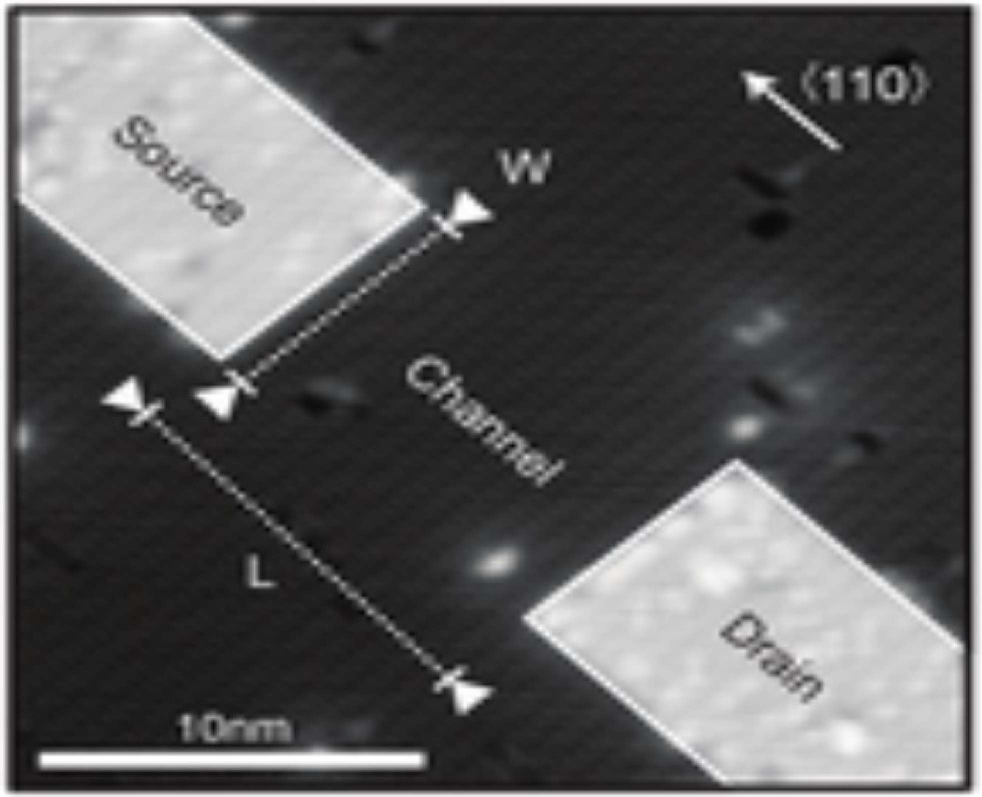
ADVANCED FUNCTIONAL MATERIALS

Research Article | Open Access

Multi-Scale Modeling of Tunneling in Nanoscale Atomically Precise Si:P Tunnel Junctions

Matthew B. Donnelly, Mushita M. Munia, Joris G. Keizer, Yousun Chung, A. M. Saffat-Ee Huq, Edyta N. Osika, Yu-Ling Hsueh, Rajib Rahman, Michelle Y. Simmons

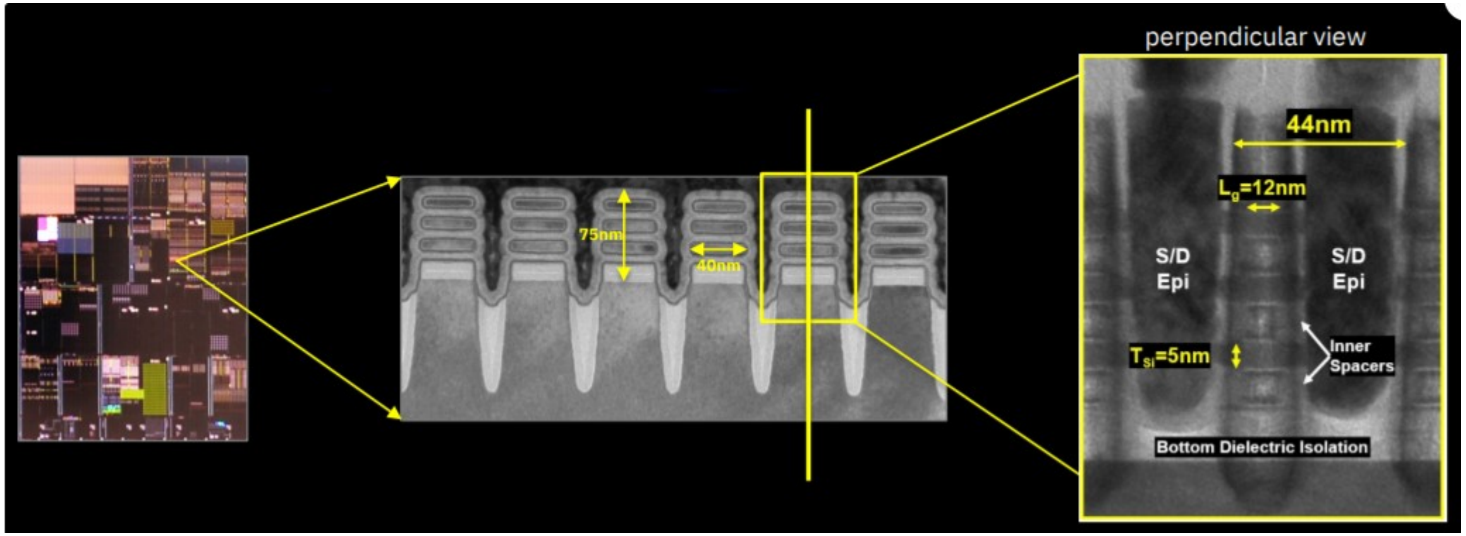
First published: 08 March 2023 | https://doi.org/10.1002/adfm.202214011



Simulations of modern GAA NSFETs with tight-binding codes are still too expensive

SILVACO/NEMO5 scaling

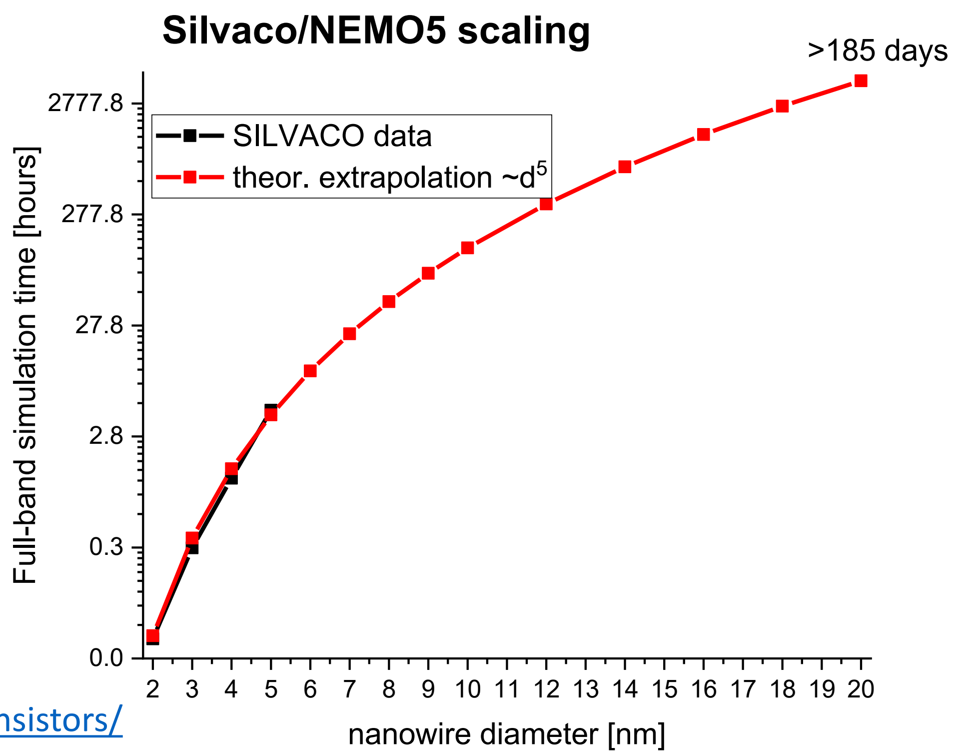
IBM, Intel and Samsung partnership*



Required simulation volume: ~ 70nm x 50nm x 30nm

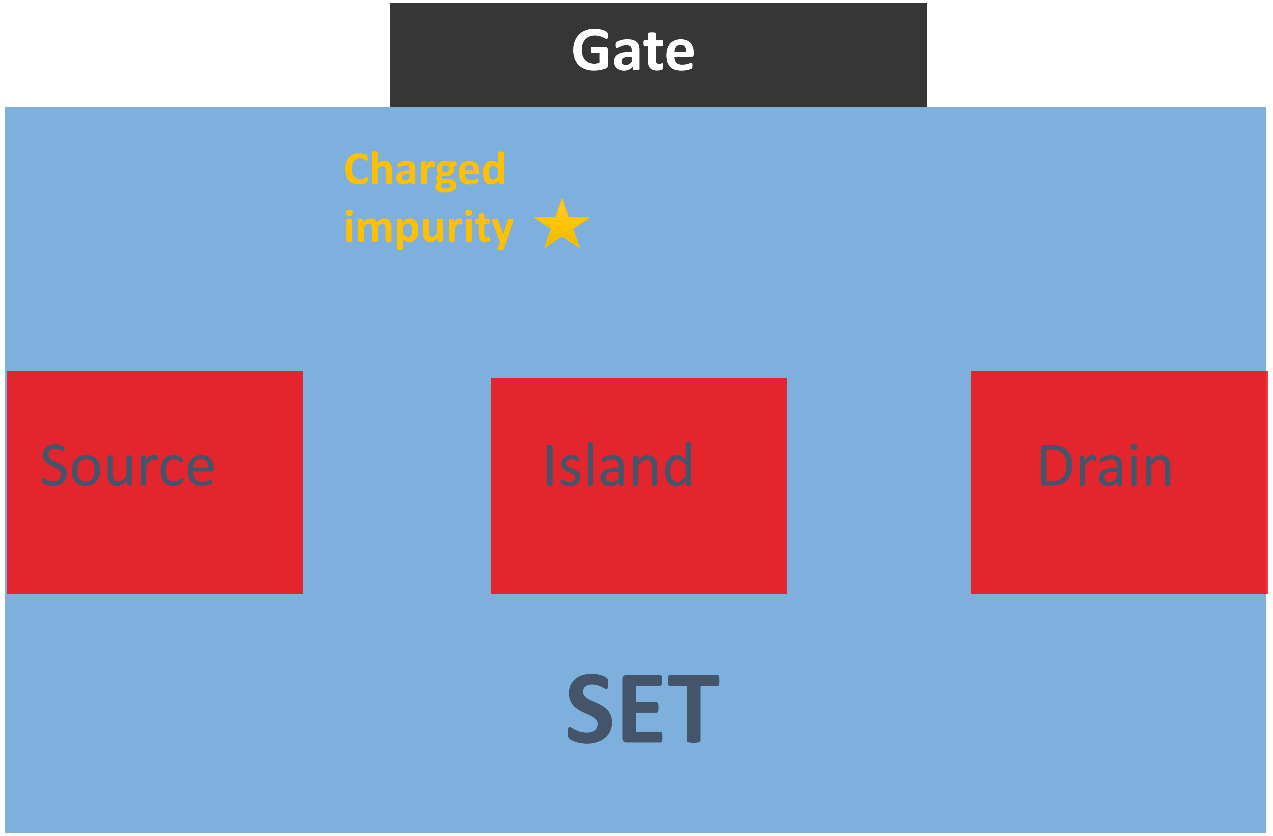
Source: "Quantum Transport Simulation at Atomistic Accuracy of a Nanowire FET",

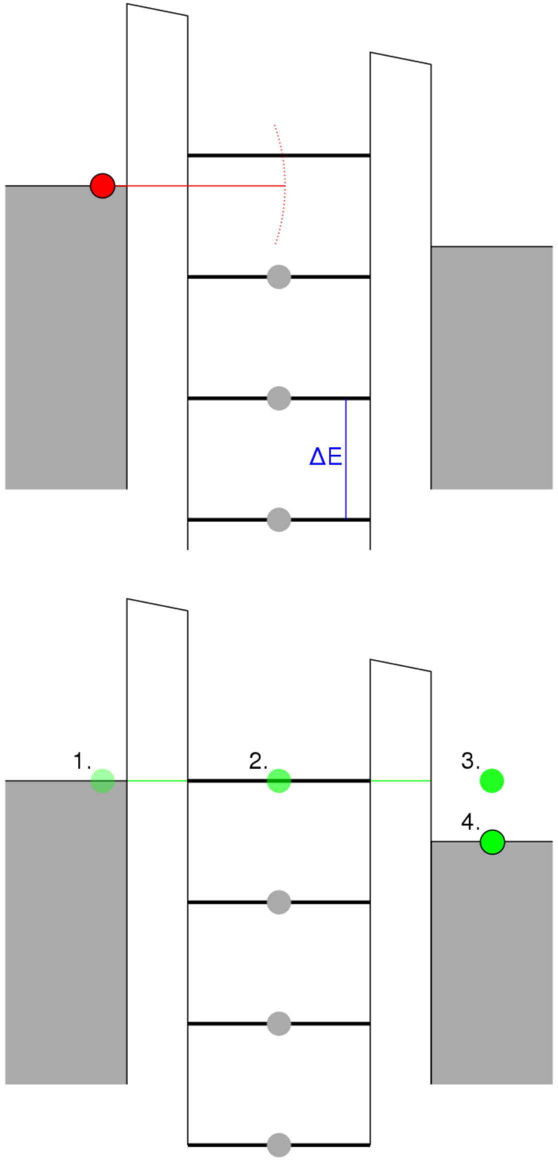
Journal for Process and Device Engineers, Volume 32, Number 8, August 2022, SILVACO



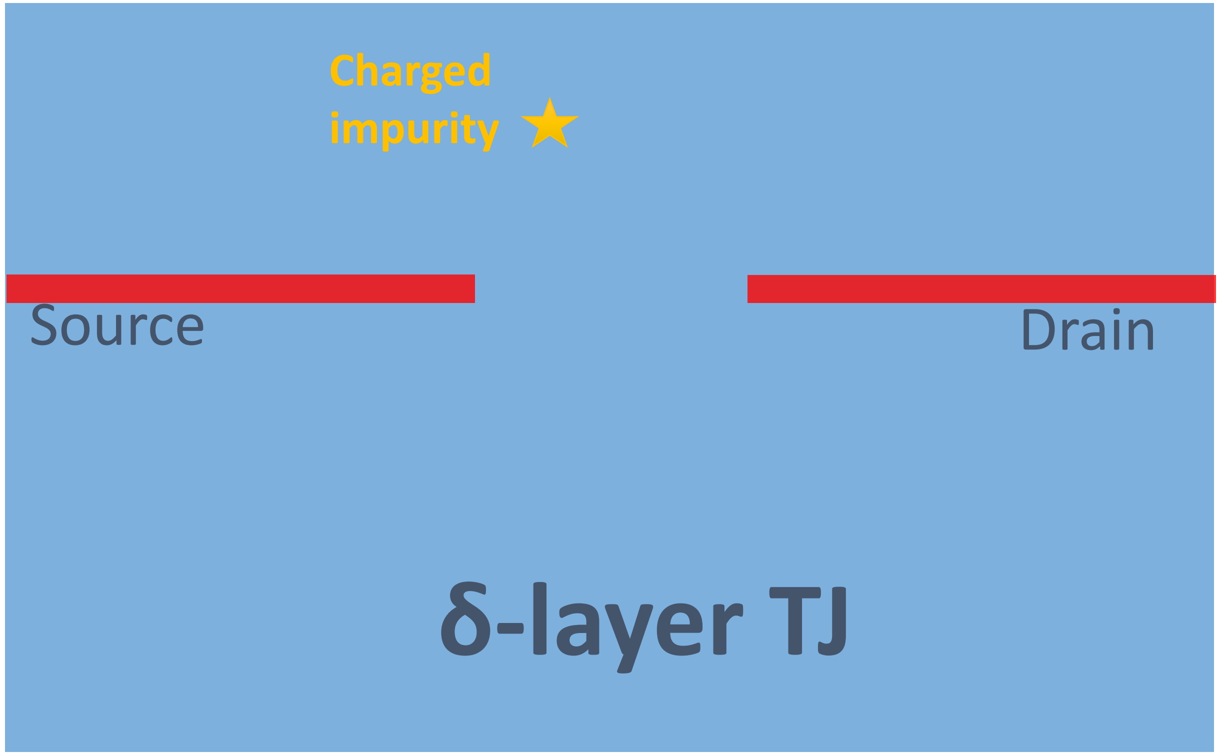
* https://www.hpcwire.com/2021/05/06/ibm-research-debuts-2nm-test-chip-with-50-billion-transistors/

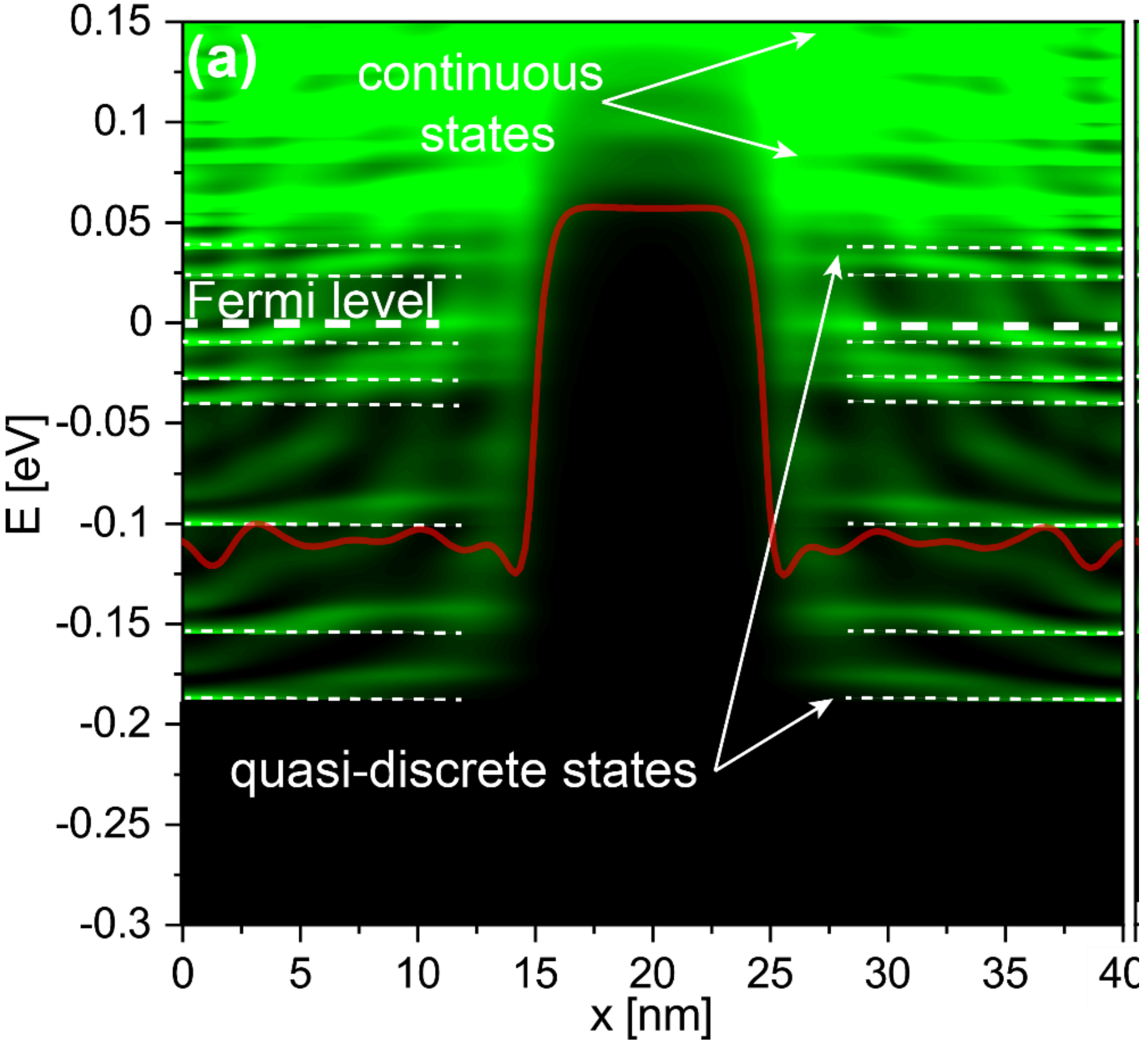
Charge sensing with SETs



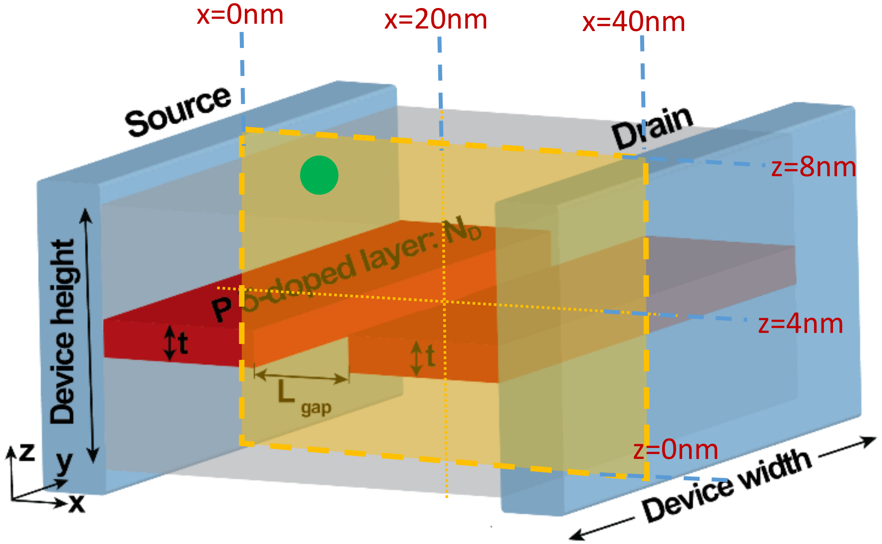


Charge sensing with δ-layer tunnel junction





δ-layer TJs are ultrasensitive to charges!



Applied voltage: 100mV
HPC Cluster: SOLO
~ 700 simulations

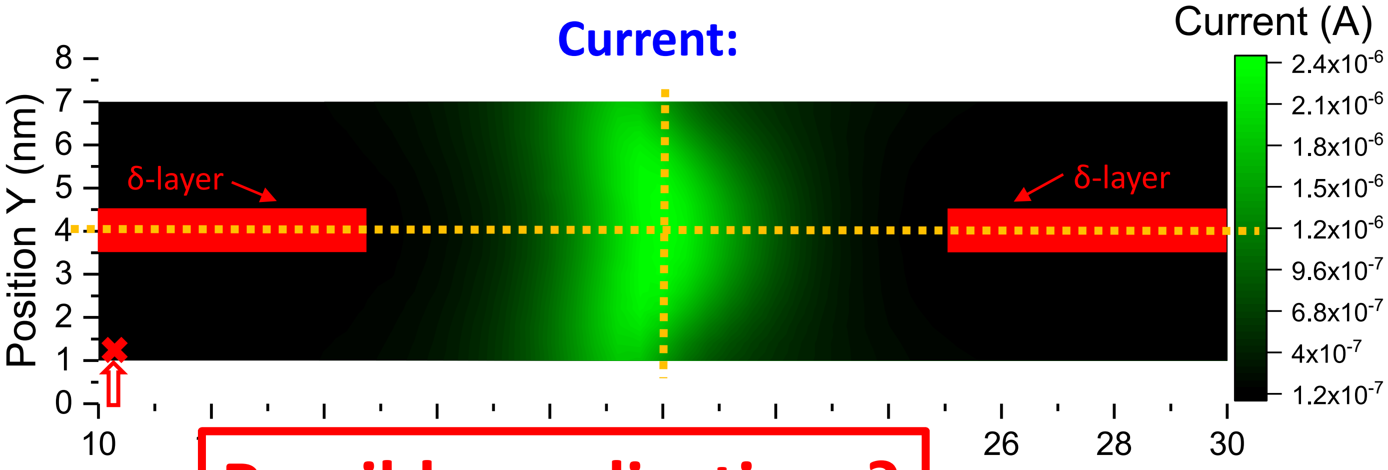

arXiv > cond-mat > arXiv:2209.11343

Condensed Matter > Mesoscale and Nanoscale Physics

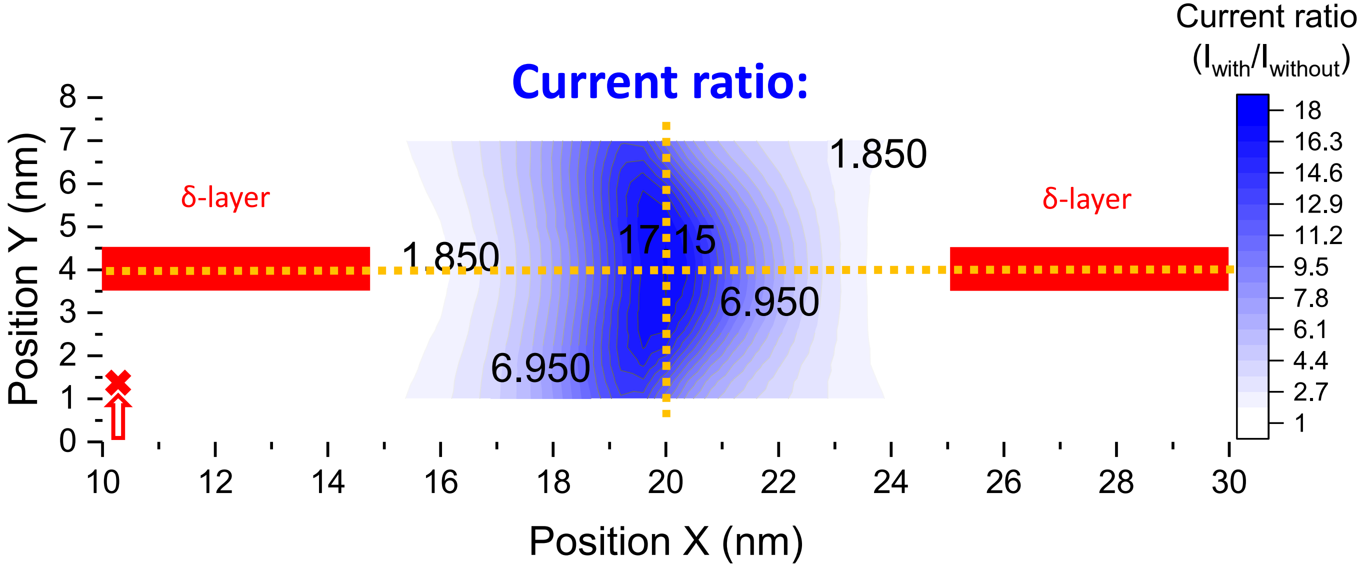
[Submitted on 22 Sep 2022]

Influence of imperfections on tunneling rate in δ-layer junctions

Juan P. Mendez, Shashank Misra, Denis Mamaluy

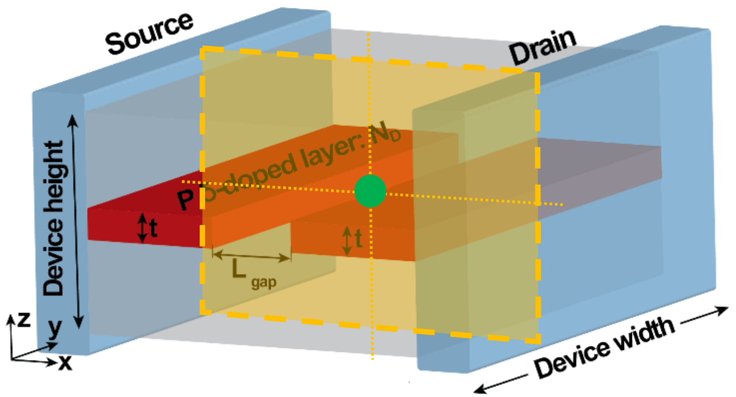


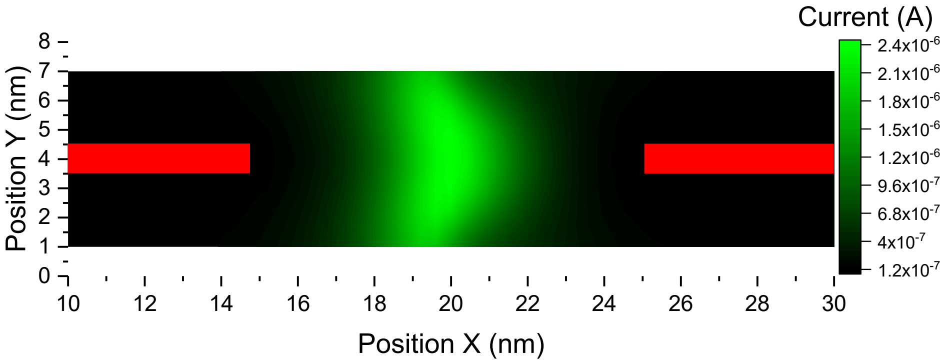
Possible applications?



δ-layer TJs are ultrasensitive to charges!

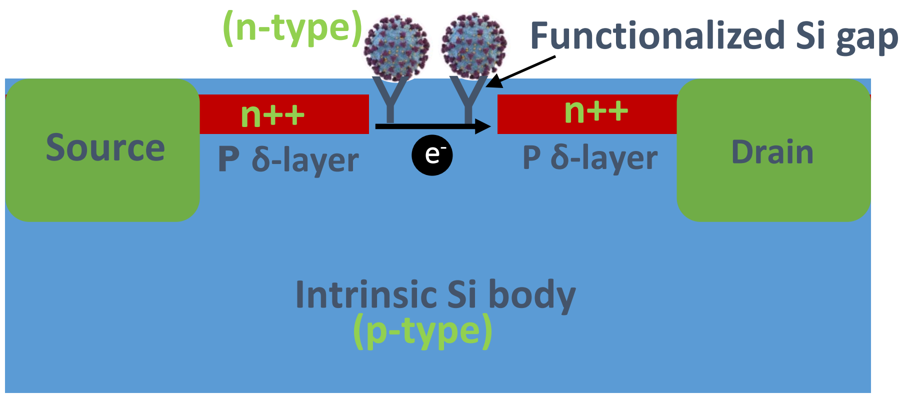
Ultrasensitive device...



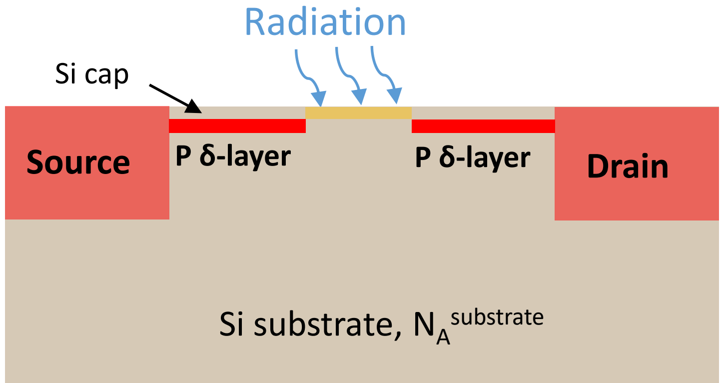


Quantum FET-based sensors

- **Chemical/Biological detection**



- **Charge Sensing at Room Temperature**



Conclusions

- 1) Highly-conducting highly-confined systems **require** an open-system treatment (e.g. NEGF) to correctly represent the number of occupied states, LDOS and current.
- 2) Kinetic energy operator with the effective mass tensor enables truly predictive *transport* simulations in silicon.
- 3) Quantum charge sensing is possible with extremely simple ("inverse-SET") structures, that are just δ-layer Tunnel Junctions. The effect is due to the conduction band quantization