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Conductive Properties of Tunnel Junctions in Semiconductor δ-layer Systems

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Please see the below presentation *first*:
"Quantum Transport Framework for Highly Conductive δ-layer Systems"

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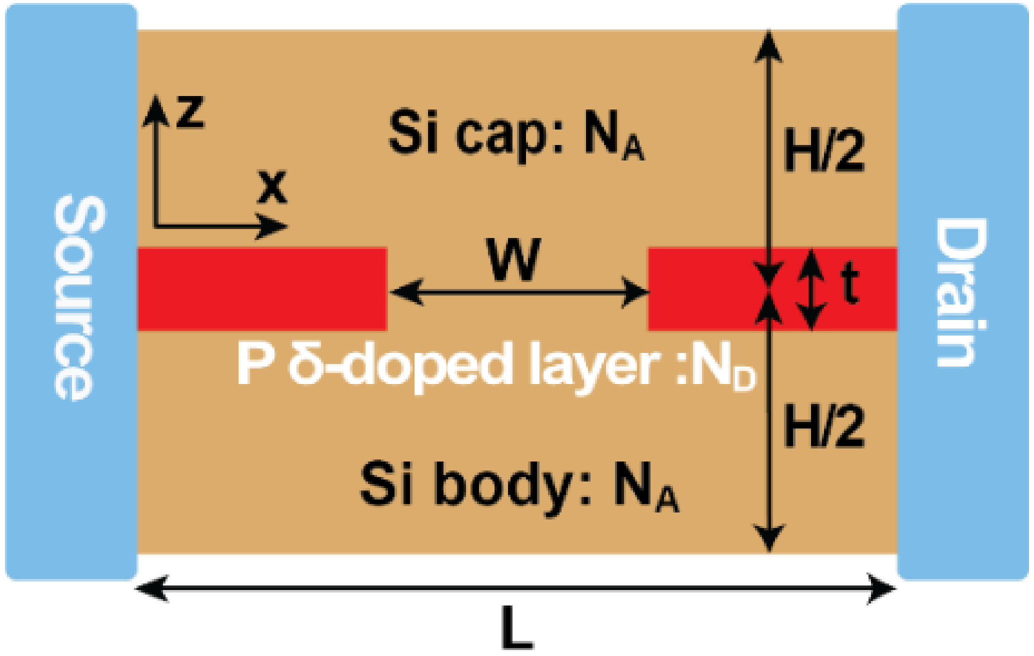
APAM Tunnel Junctions



Si: P δ-layer Tunnel Junction

- DOS are *practically* the same for all W
- Current/conductivity orders of *magnitude* different!
- An illustration that DOS =/= Flux *while LDOS (density matrix) determines T(E), DOS does not*

Motivation

- We now understand (and importantly – can reproduce experiments) conduction band structure and conductive properties of Si: P δ-layer wires

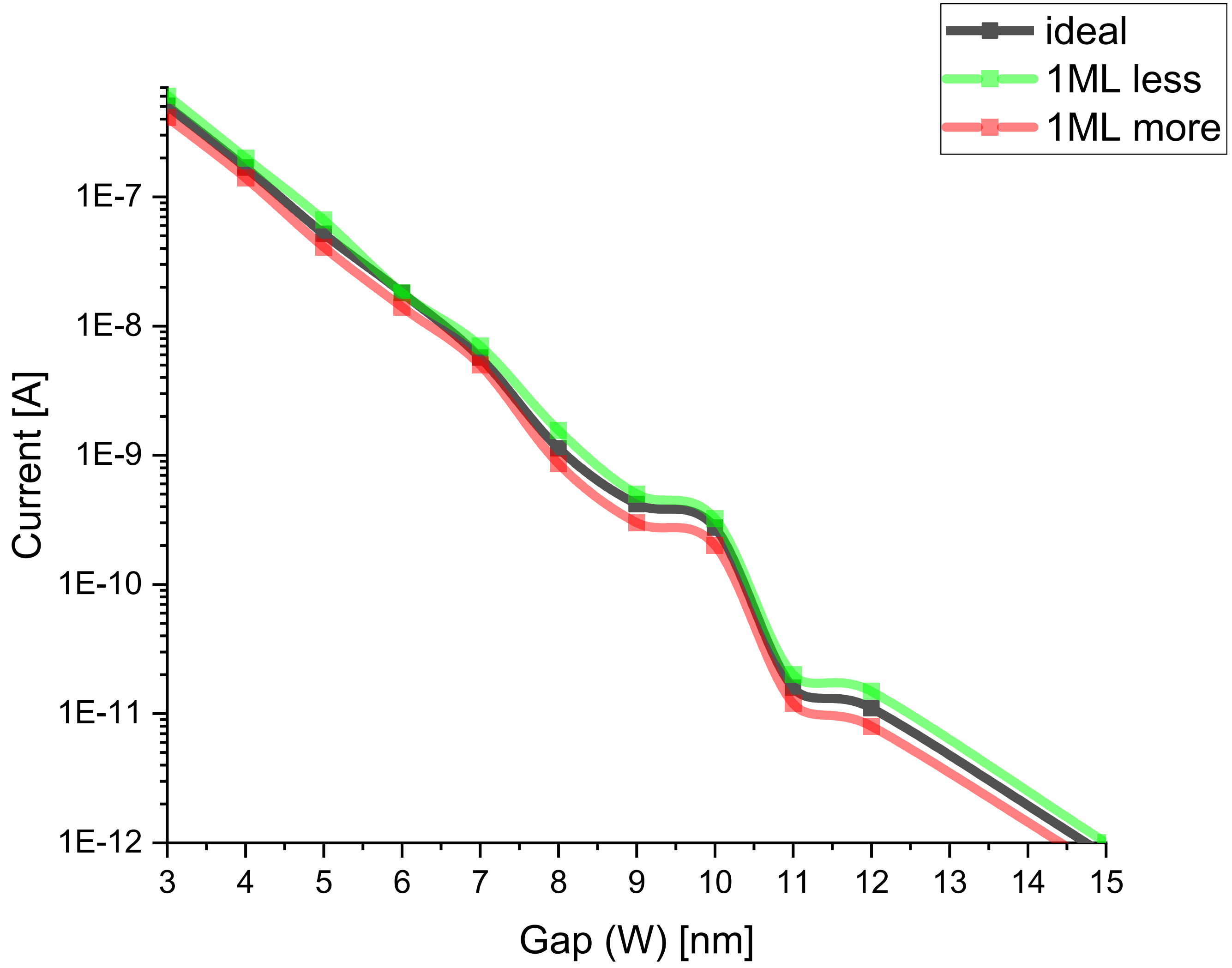
  D. Mamaluy, *et al*, Submitted to Comm. Phys. (Feb. 2021)

- The next logical step – consider tunnel junctions (TJ)
- Unlike with the wire conduction analysis, there have been a few previous attempts to study such δ-layer systems theoretically
- Reasons: From QM point of view, TJs can only be analyzed with the help of open-system treatments (such as NEGF); periodic BC are just not applicable

Open system treatment of TJ: why hard?

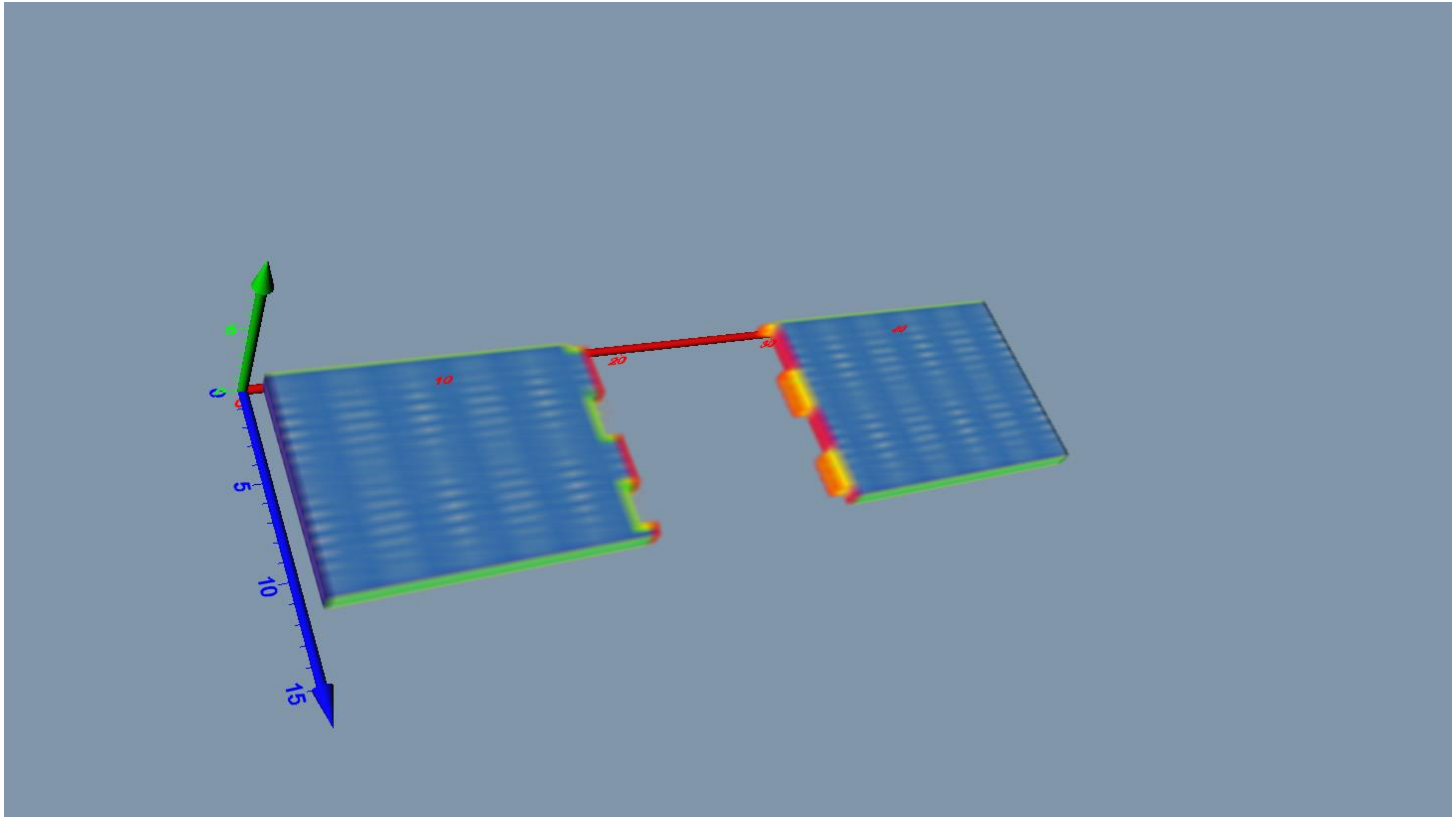
- NEGF solves open-system Schrodinger equation
- Solutions are continuous in energy (not eigenstates!)
- NEGF generally scales as $O(N^3)$ with the system size N
- For realistic systems, such as TJs, N ~ 10^5-10^7
- NEGF is a hard problem to solve and $O(10^{15}$-$10^{21})$ operations needs to be performed repeatedly to achieve the charge self-consistency
- Not doable even with the modern supercomputers

Current vs ideal gap width (W)

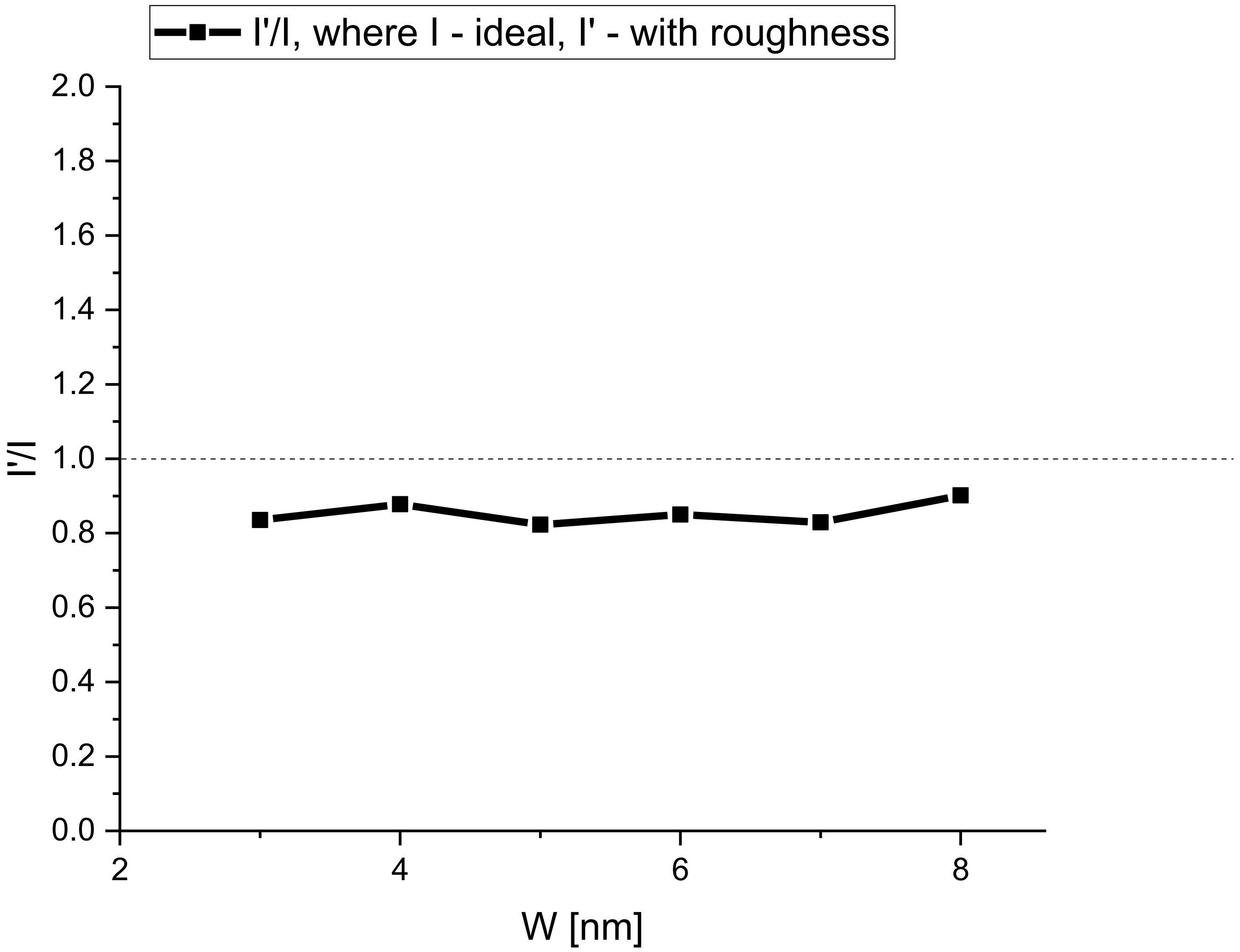


- I vs W trend is exponential up to 15 nm
- Observable quantum effect around 10 nm due to geometry

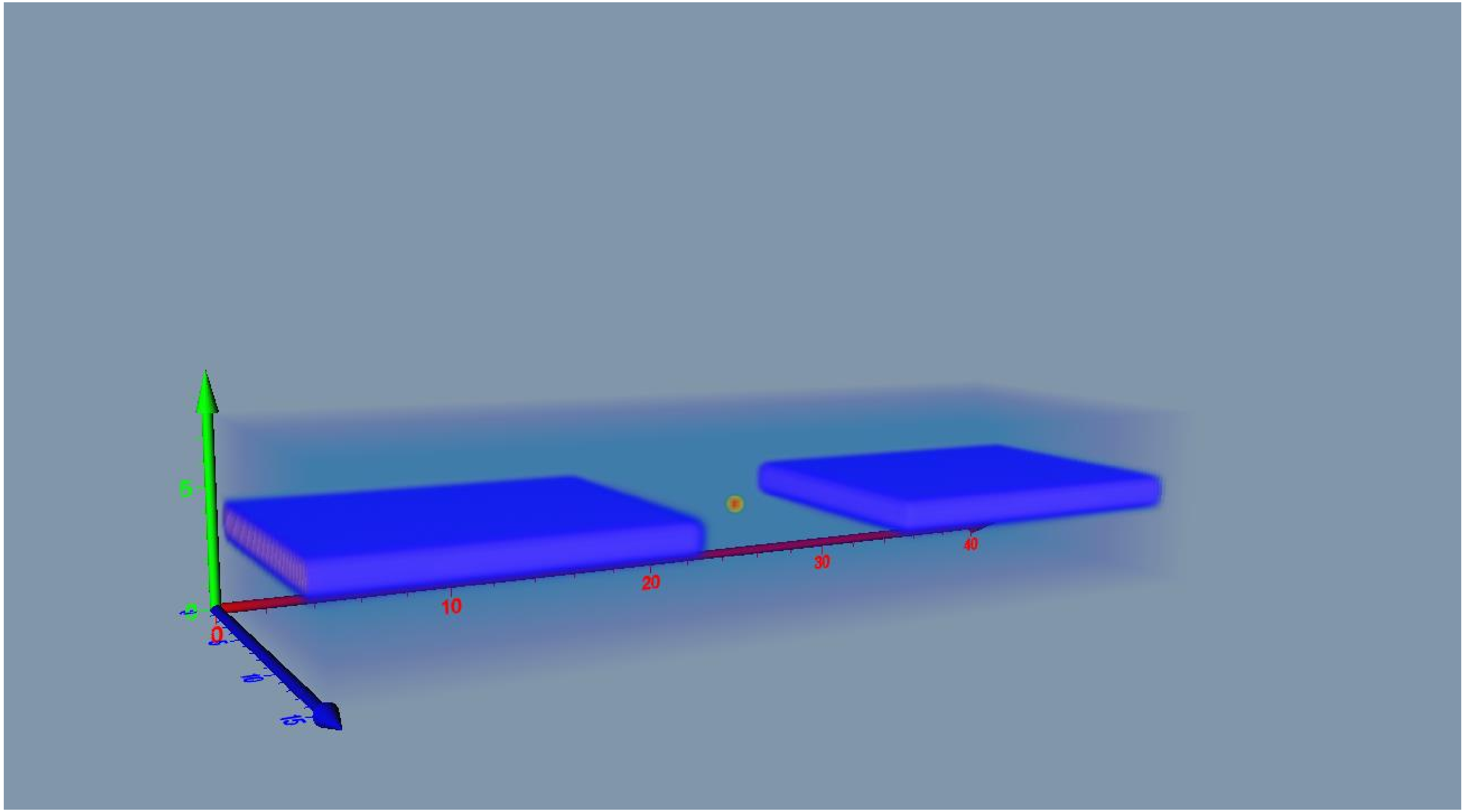
Gap roughness emulation



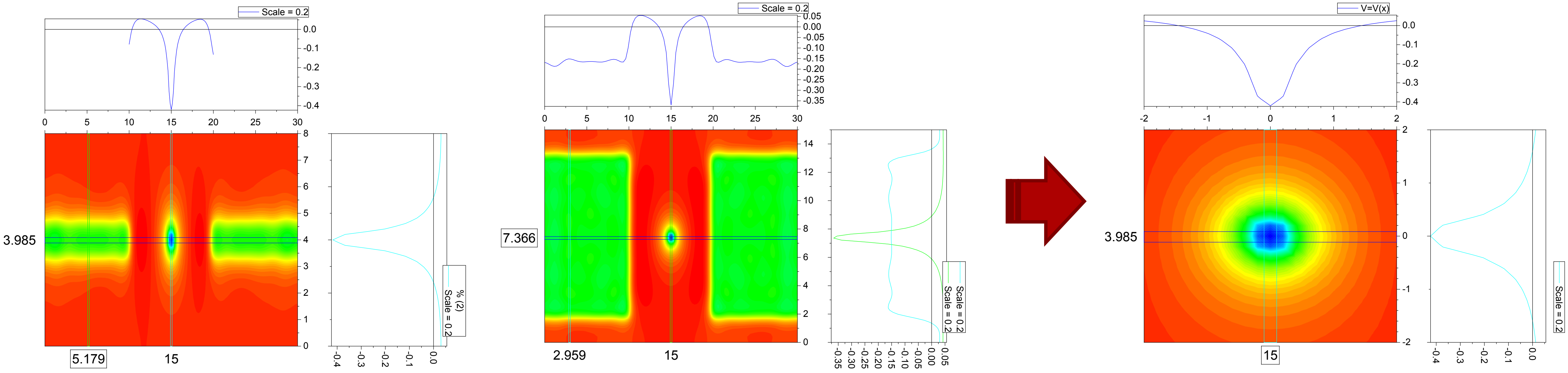
Gap roughness reduces current by about 20%!



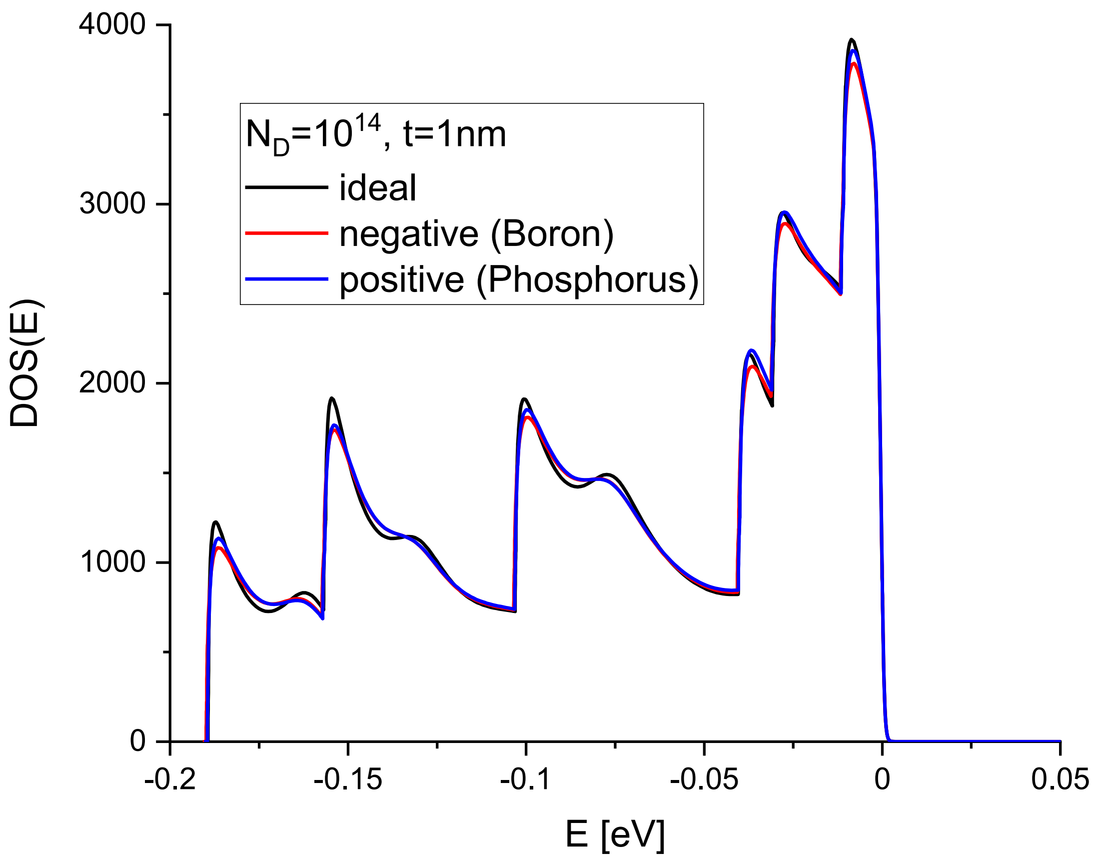
A charged impurity in the gap

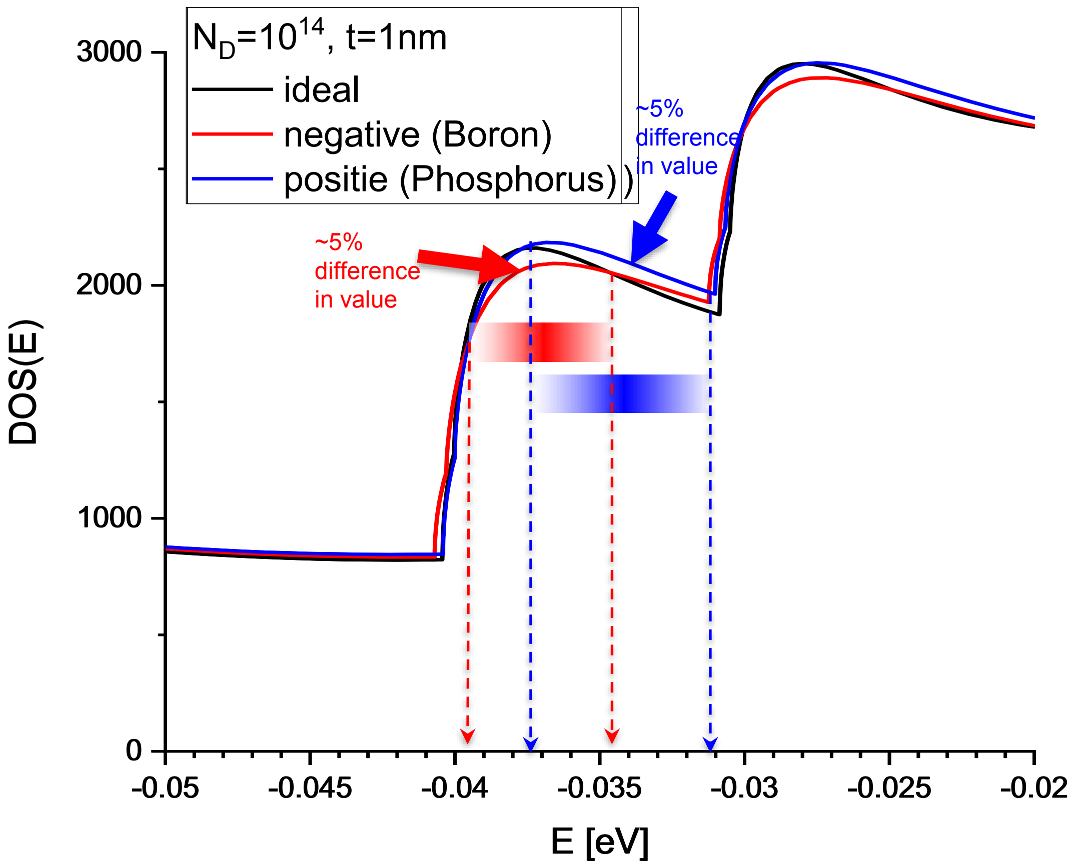


Discrete charge emulation details

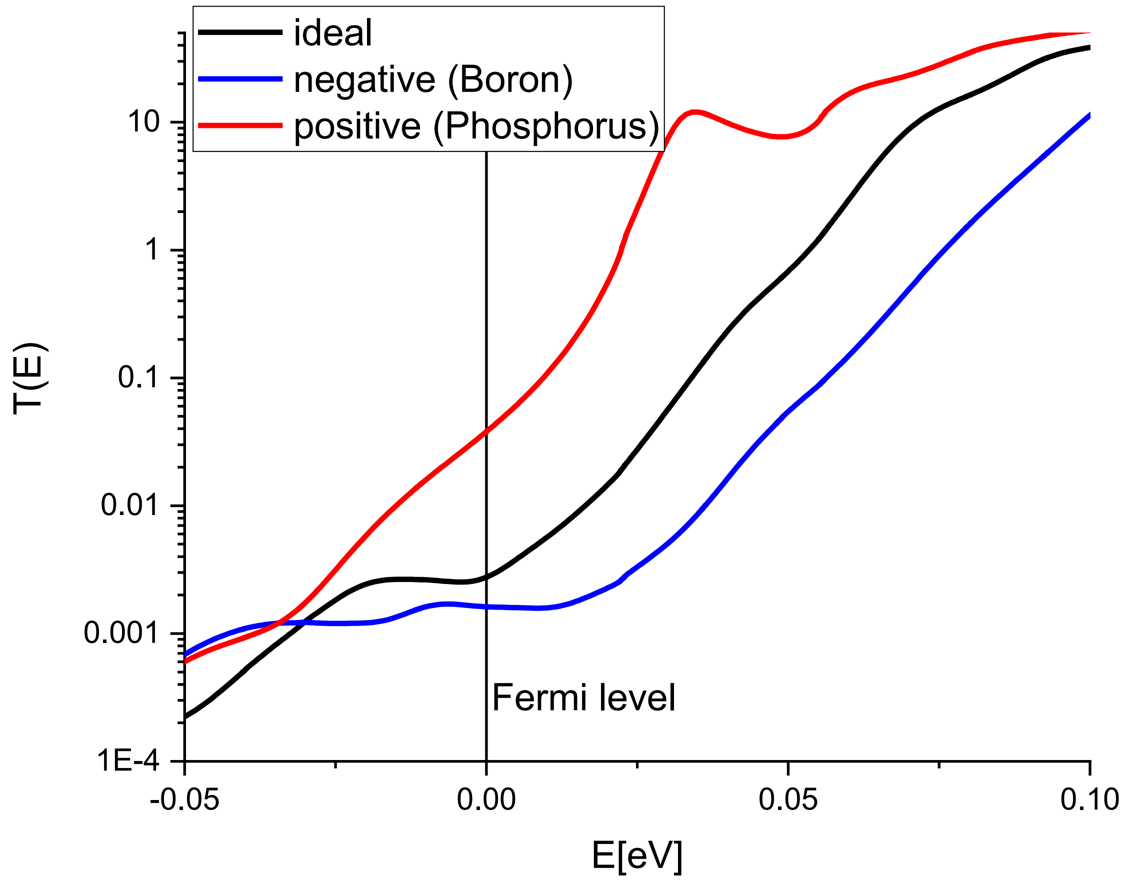


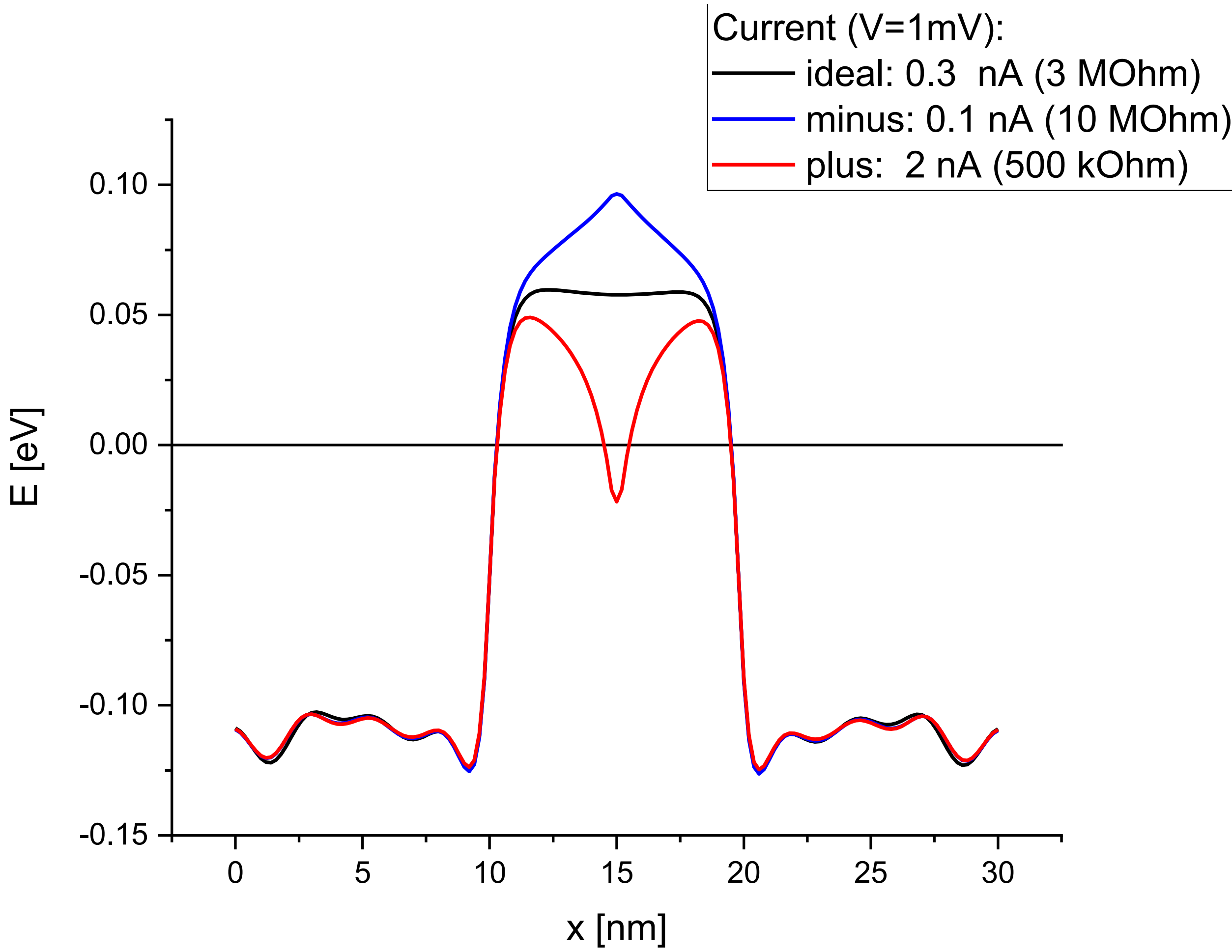
Density of states: spectroscopy detection?



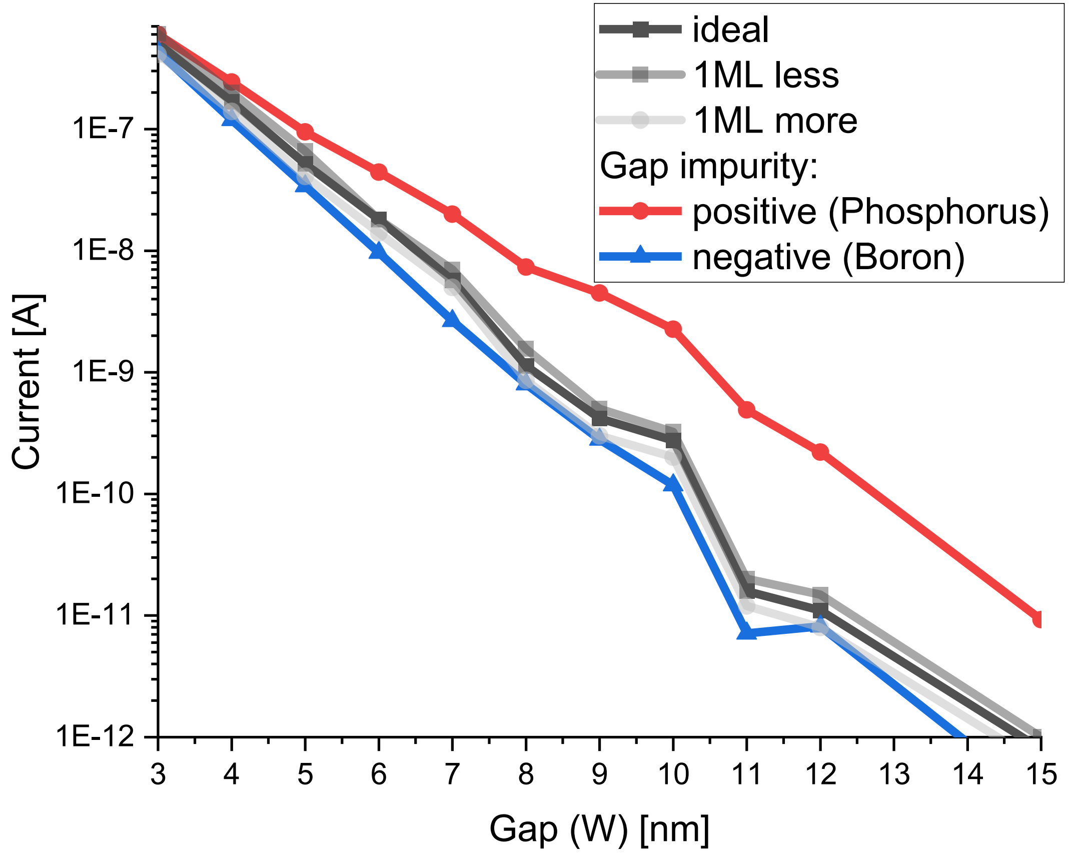


Transmission function: does a gap impurity matter?





A single charged impurity in the gap!



- **Asymmetric behavior with the impurity electrical sign:** positively charge impurities dramatically affect the current value, increasing the current by an order of magnitude; negatively charged impurities reduce the current in a significantly smaller manner.

Summary

- Charge self-consistent NEGF is a proper tool to study conductive properties of devices and materials
- TJs: I vs W is roughly exponential up to W=12nm
- Gap roughness reduces the current by about 20%
- A single charged impurity in the TJ gap can dramatically affect the current
- A negative impurity (Boron) reduces the current by a factor of 2
- A positive impurity (Phosphorus) increases the current by an order of magnitude!

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