

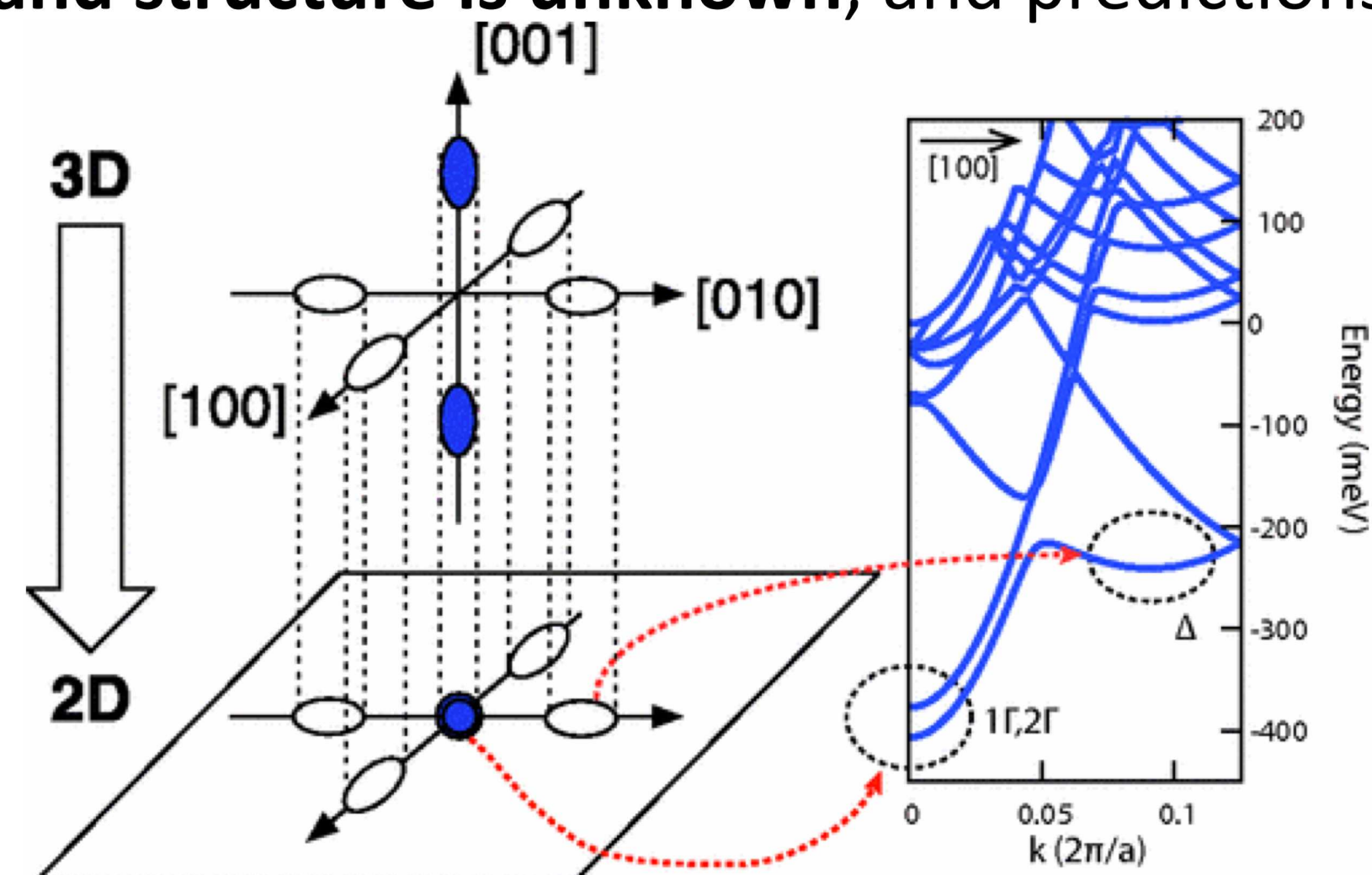


Modeling Transport in Phosphorus δ -Doped Silicon Tunnel Junctions

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Opportunities and Mysteries of Phosphorus δ -Doped Silicon

Opportunity to **fabricate electrical devices with atomic precision**. Electrons are confined to a 2D sheet by a highly doped ($\approx 1.7 \times 10^{14} \text{ cm}^{-2}$) monolayer of P. The resulting **band structure is unknown**, and predictions vary substantially.

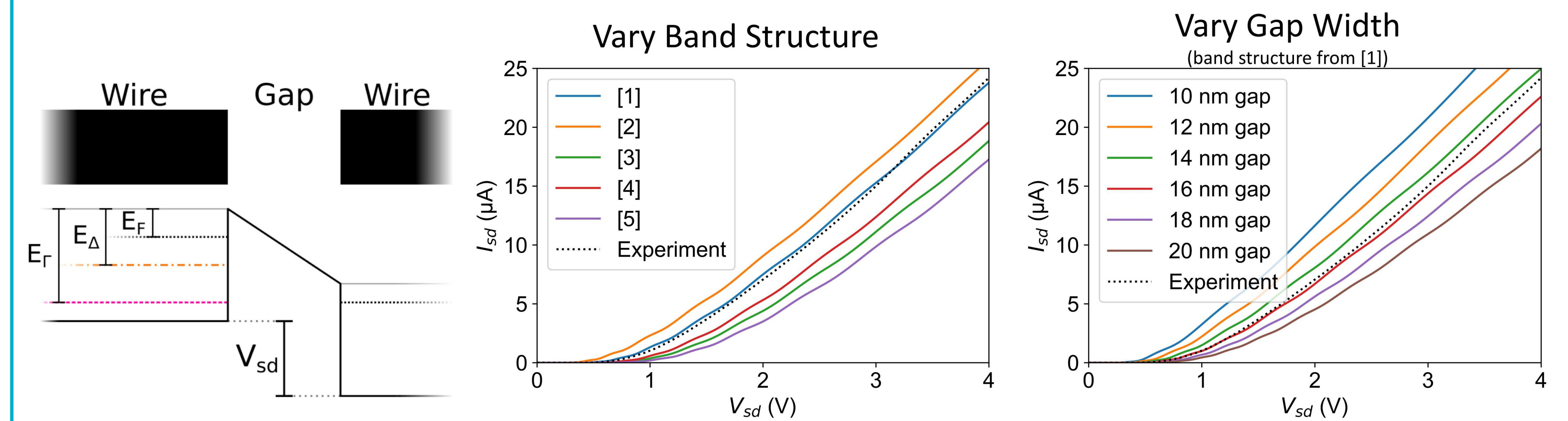


Model	E_{Γ_1}	E_{Γ_2}	E_{Δ}	E_F
DFT (1D) [1]	296	288	165	72
DFT (3D) [2]	369	269	68	23
TB (3D) [3]	401	375	249	115
DFT (1D) [4]	419	394	250	99
TB (3D) [5]	427	421	287	142

Figure from S. Lee et al., Phys. Rev. B, **84**, 205309 (2011).

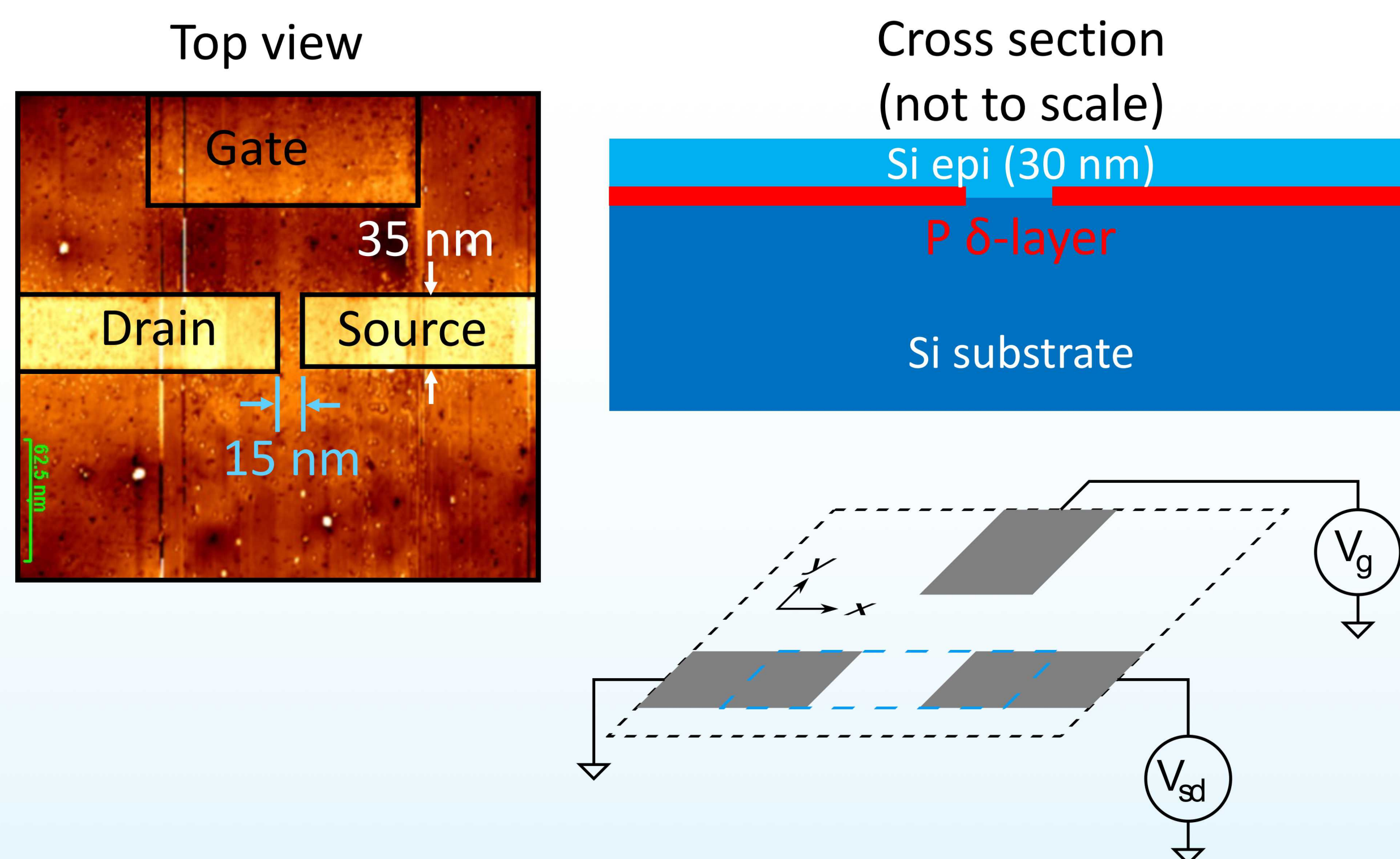
1D Model: Band Structure Revealed?

Trapezoidal barrier model of tunnel junctions produces reasonable results and shows impact of band structure. **One band structure fits experimental results** (assuming 78 k Ω series resistance). However, **small variations in gap width have comparable effects**.



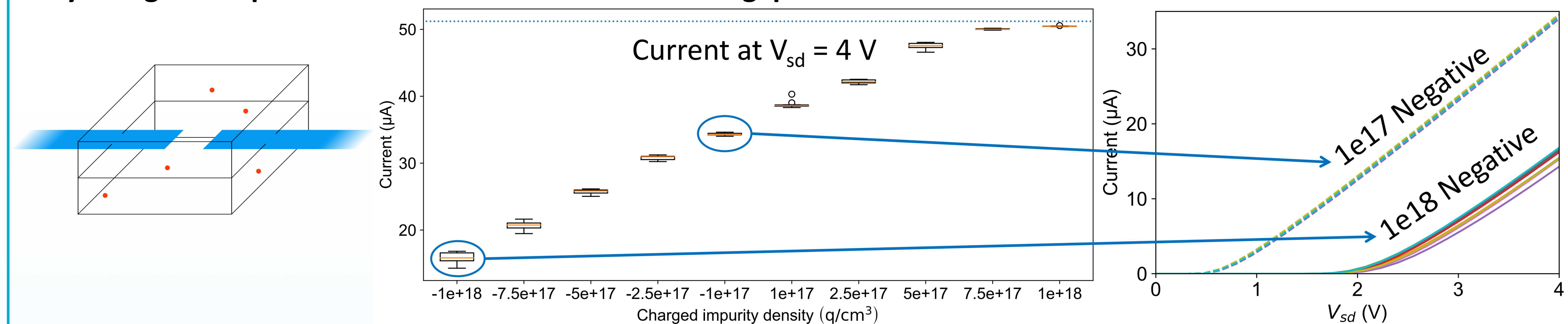
δ -Doped Silicon Tunnel Junctions

STM lithography allows us to pattern δ -layers into devices with atomic precision. For testing fabrication and models, we have made a variety of tunnel junctions. Will consider below design.



Stray Charges as Spoilers

Epi layer contains many stray charges, which requires a more advanced model. Electrostatics with boundary element method and 2D transport with Kwant [6]. 10 runs with randomly placed charges for each stray charge density. **Effect of stray charges comparable to band structure choice and gap.**



Conclusions

- Simple models are promising way to understand δ -doped devices
- Stray charges have effects comparable to band structure choice
- Imperfections in geometry also important
- Several good junctions could nail down the band structure

References:

1. D. J. Carter et al., Nanotechnology, **22**, 065701 (2011).
2. D. W. Drumm et al., Nanoscale Res. Lett., **8**, 111 (2013).
3. H. Ryu et al., Nanoscale, **5**, 8666 (2013). S. Lee et al., Phys. Rev. B, **84**, 205309 (2011).
4. G. Qian et al, Phys. Rev. B, **71**, 045309 (2005).
5. J. S. Smith et al., Phys. Rev. B, **89**, 035306 (2014).
6. Groth et al., New J. Phys., **16**, 063065 (2014).