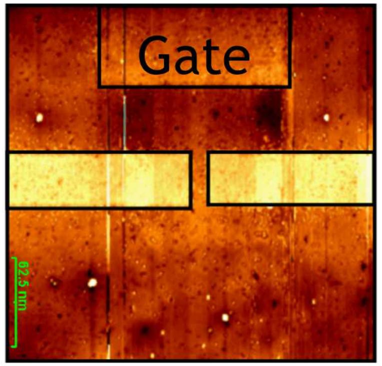
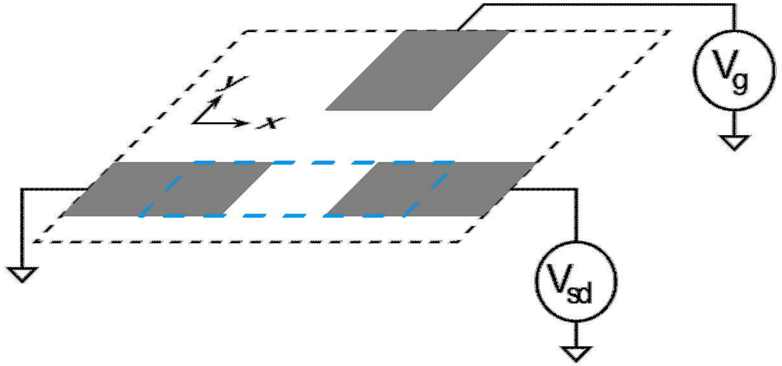
SAND2019-2247C

Modeling transport in phosphorus δ-doped silicon tunnel junctions





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Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This work was funded by the Laboratory Directed Research and Development Program.

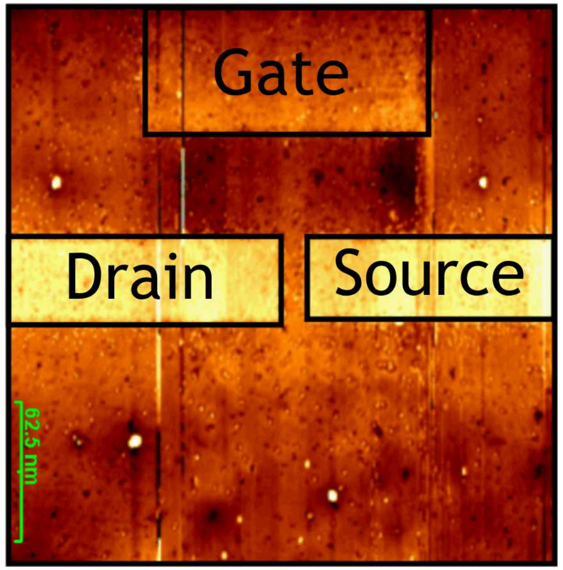
Background

- STM Lithography can produce atomically precise, 2D layers with extremely high doping (1.7e14 cm^{-2}) in Si
- Potential use in fabricating a variety of electrical devices
- Very high doping -> does not act like normal Si!
- Requires relatively low fabrication temperatures -> tricky fabrication
- Currently making test structures, including tunnel junctions, to better understand fabrication and δ-layer properties
- Investigating:
  - Simple models for transport
  - Effects of impurities

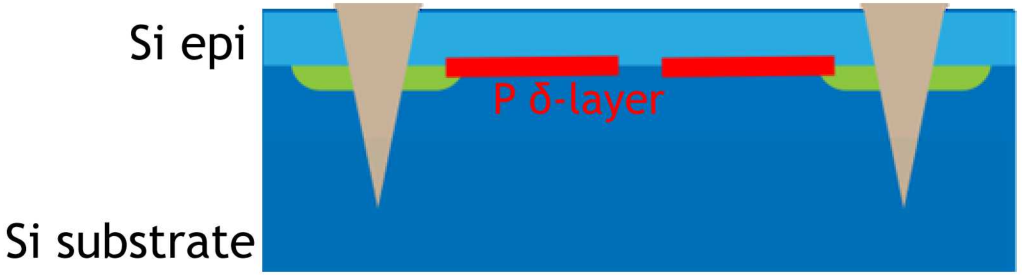
STM lithography and δ-layers

- Technique pioneered by Lyding and Simmons, now also done at Sandia and NIST
- STM lithography gated tunnel junction shown
- Fast fabrication facts
  - Uses hydrogen attached to Si substrate as a mask
  - P attached to ~1/4 of unmasked Si (~1.7e14 P atoms/cm-2)
  - 30 nm of epitaxial Si grown on top
- P confined to few-monolayer-thick "δ-layer"

Top View



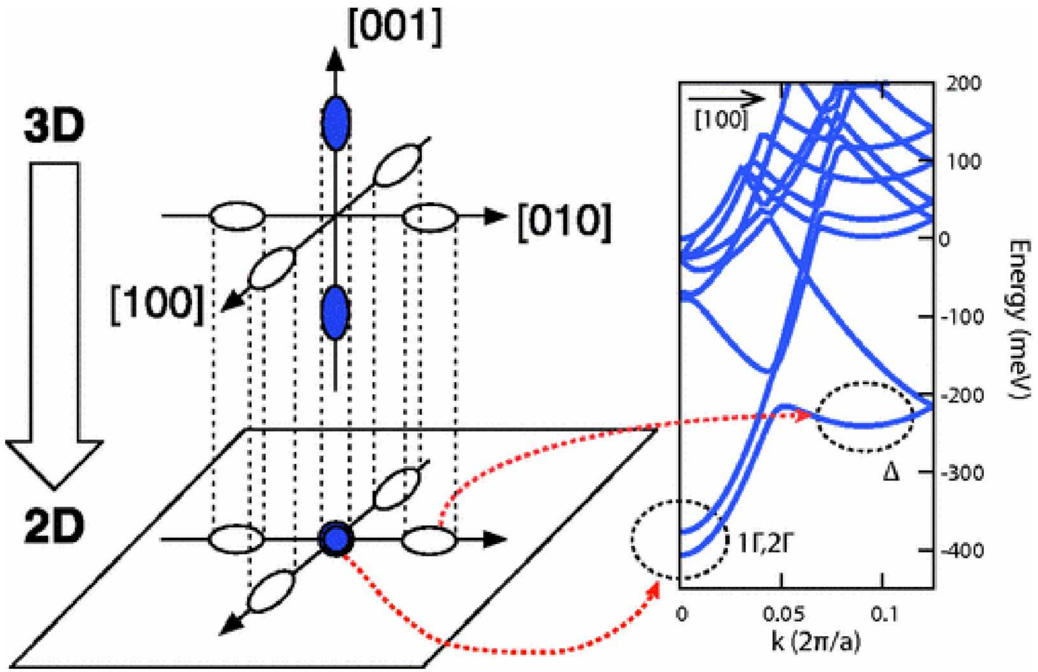
Cross section of TJ



J. W. Lyding et al., Appl. Phys. Lett., **64**, 2010 (1994).
T. Hallam et al., J. Appl. Phys., **102**, 034308 (2007).

Mysterious properties of phosphorus δ-doped silicon

- Not bulk Si band structure!
- Hard to measure band structure of buried, disordered alloy
- Table: predicted band minima and Fermi level for quarter-layer doped δ-layer sheets (meV below Si conduction-band minimum)
- No consensus!

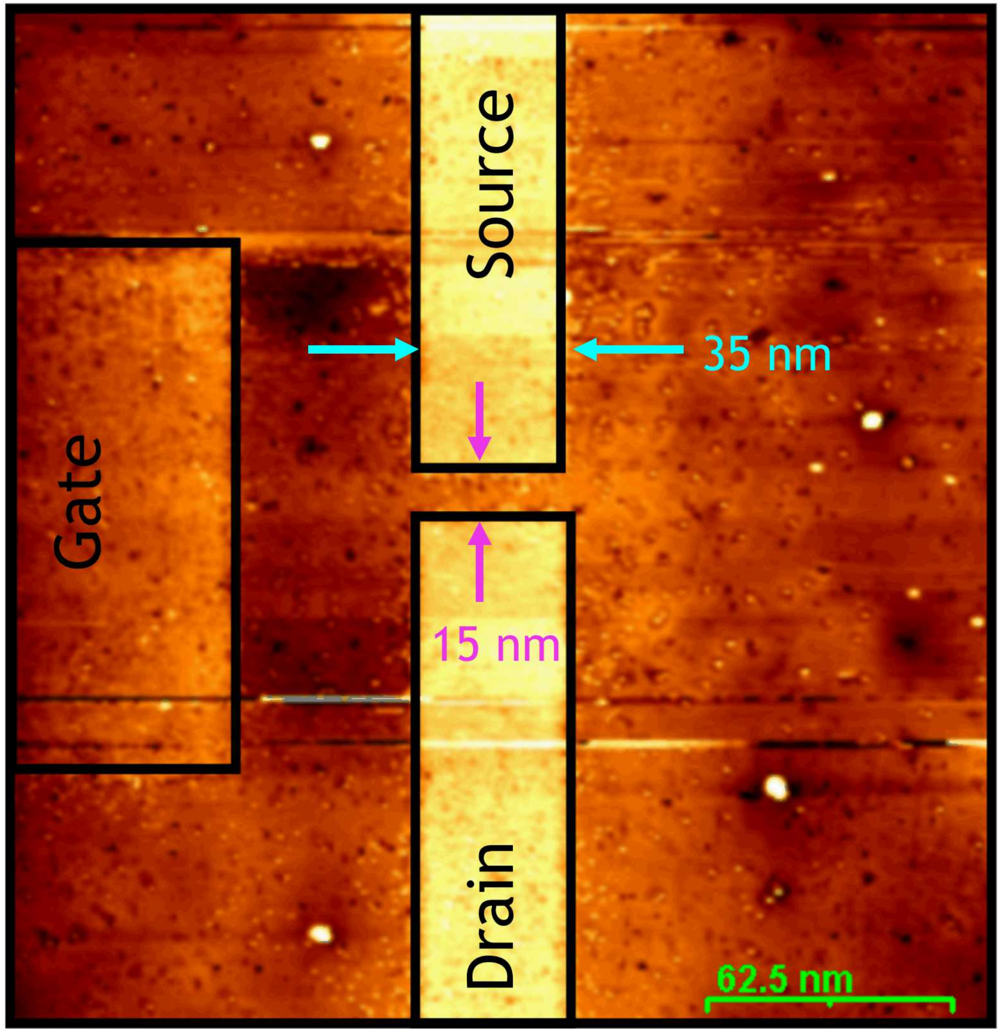


Model	E_{Γ_1}	E_{Γ_2}	E_{Δ}	E_F
DFT (1D) [1]	296	288	165	72
DFT (3D) [2]	369	269	68	23
TB (3D) [3]	401	375	249	115
DFT (1D) [4]	419	394	250	99
TB (3D) [5]	427	421	287	142

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).

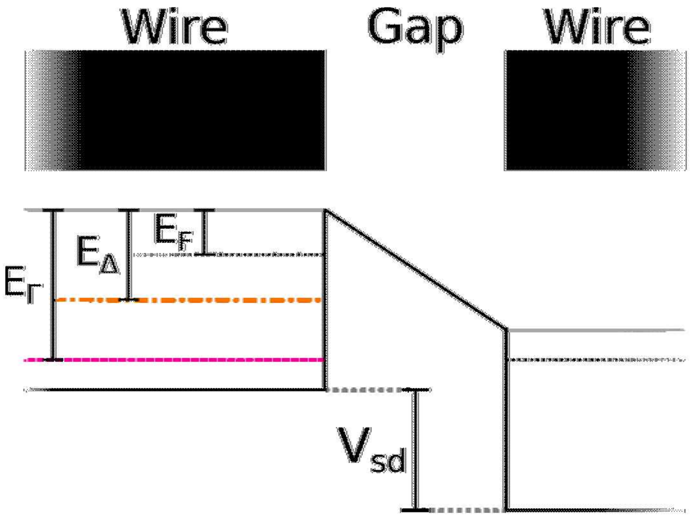
Our tunnel junctions

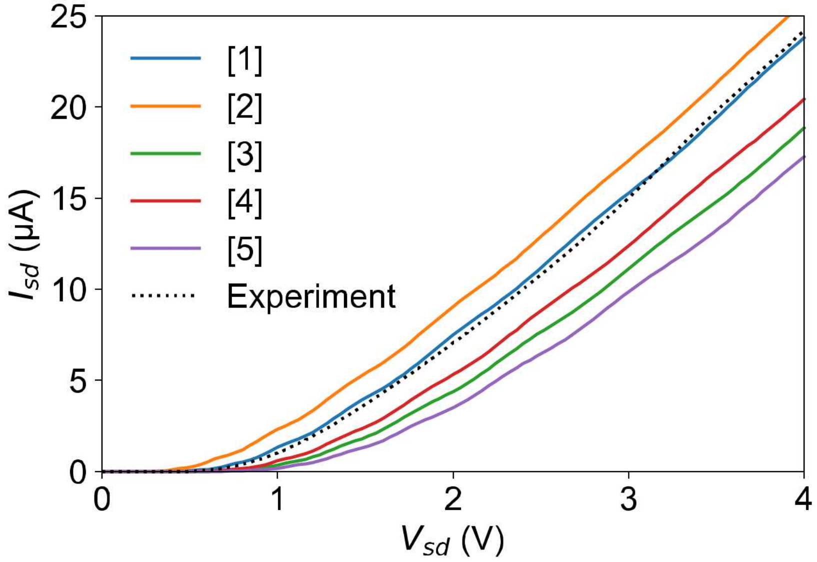
- Useful for testing fabrication and models
- Can be made with or without inplane or top gate
- Consider 35-nm-wide wire with a 15-nm-wide gap
- Effective mass theory for electrons



One-dimensional model: band structure revealed?

- Trapezoidal barrier from linear voltage drop and band offsets
- Calculate transmission/currents for all bands
- I-V curves for all parameters in Table as well as experimental data (dotted). 78 kΩ resistance in series
- Takeaways:
  - Even simple model produces reasonable results
  - Band structure matters
- Does this mean we now know the band structure?

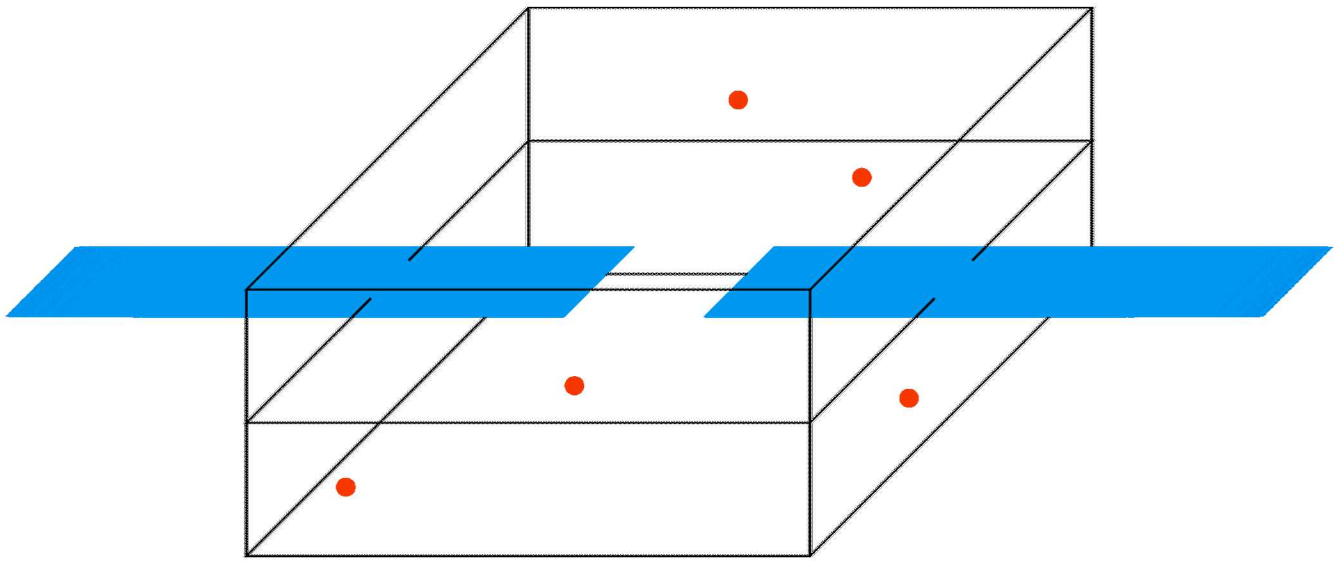




A. Shirkhorshidian et al., Phys. Rev. Appl., **10,** 044003 (2018).

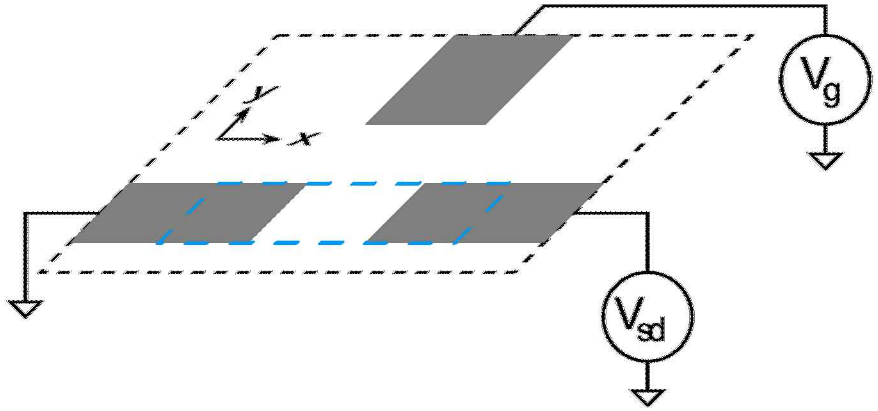
Stray charges

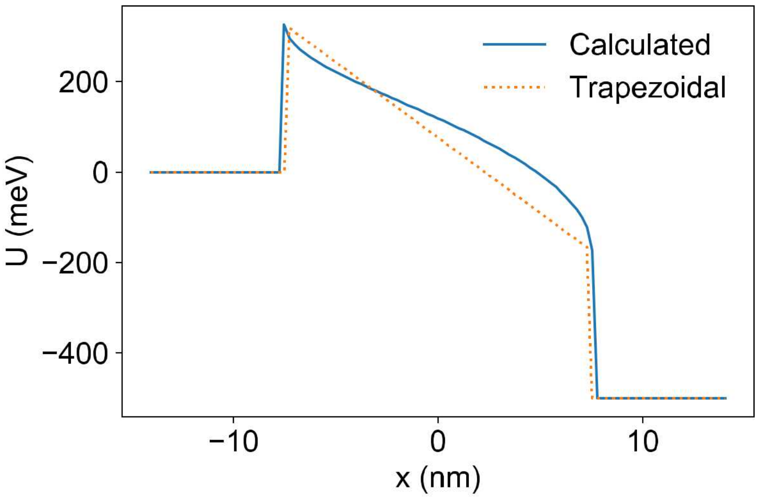
- Unfortunately, devices have defects
- Concerned with stray charges in Si grown above δ-layer
- Need model that can handle real electrostatics, including randomly located stray charges near the junction

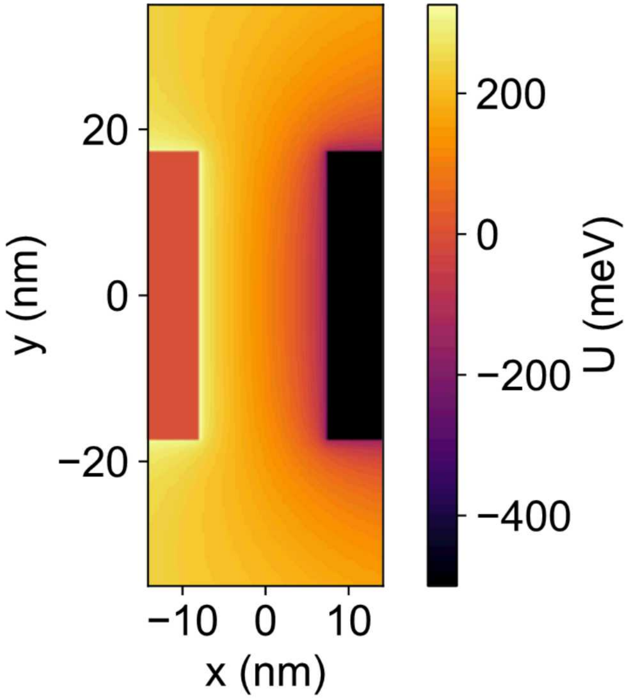


Two-dimensional model with electrostatics

- Treat δ-doped regions as perfect conductors, partially screen stray charges
- Electrostatics with boundary element method
- Kwant package to calculate transmission
- 78 kΩ resistance and band structure from [1]
- Can also include gates



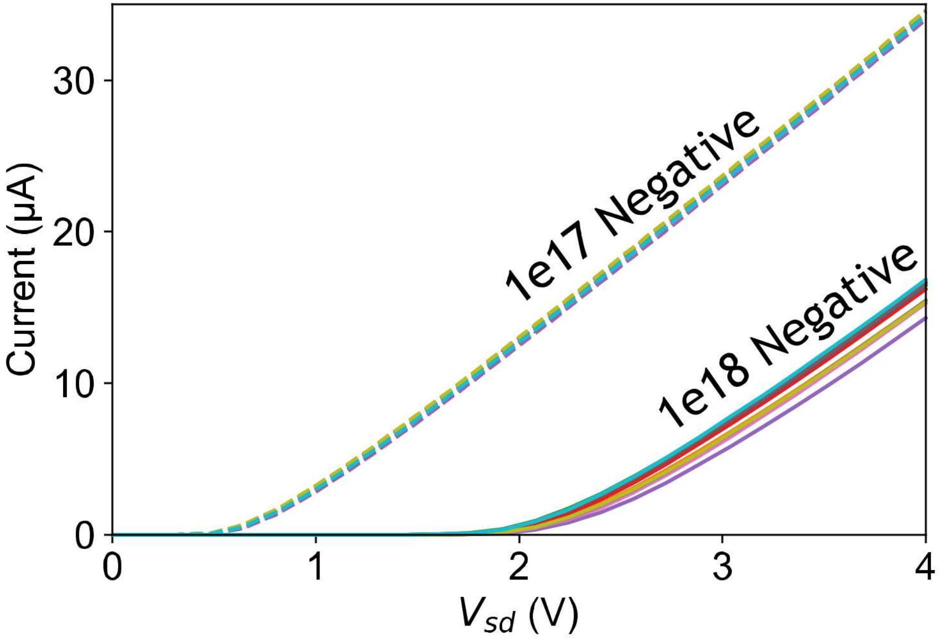


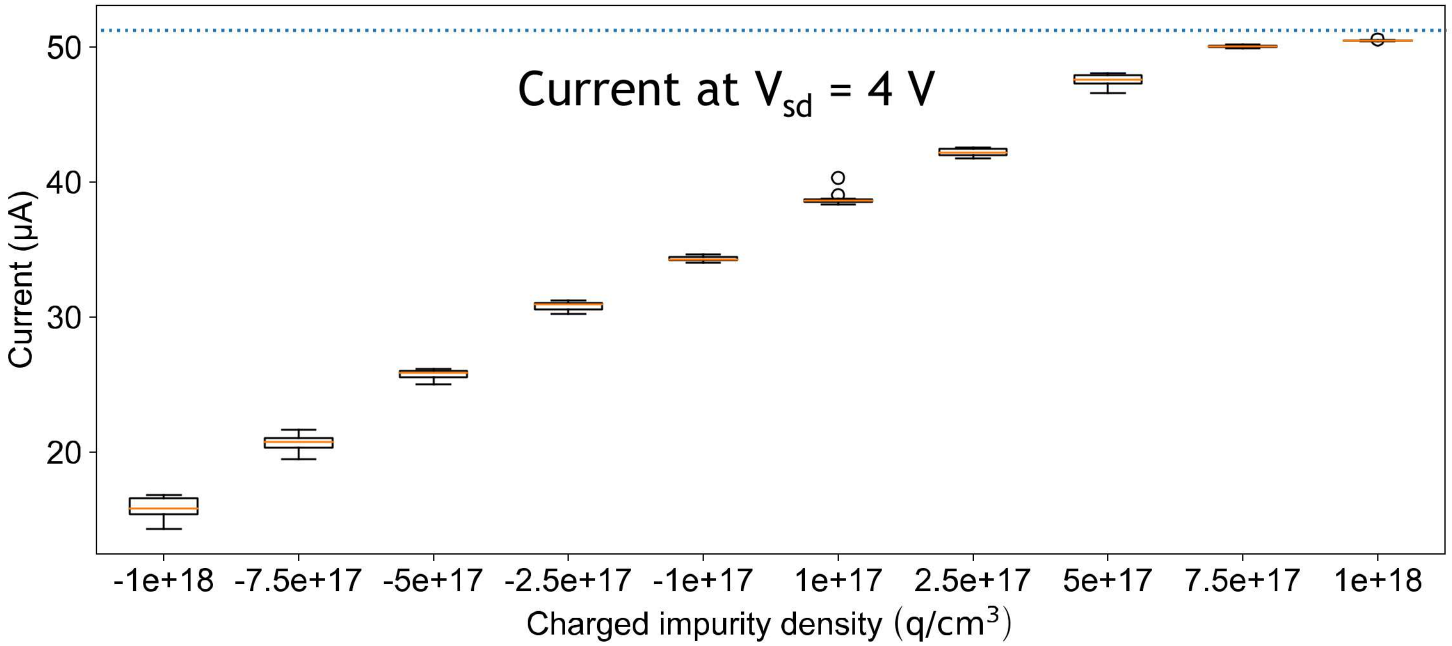


Groth et al., New J. Phys., **16**, 063065 (2014).

Stray charges as spoilers

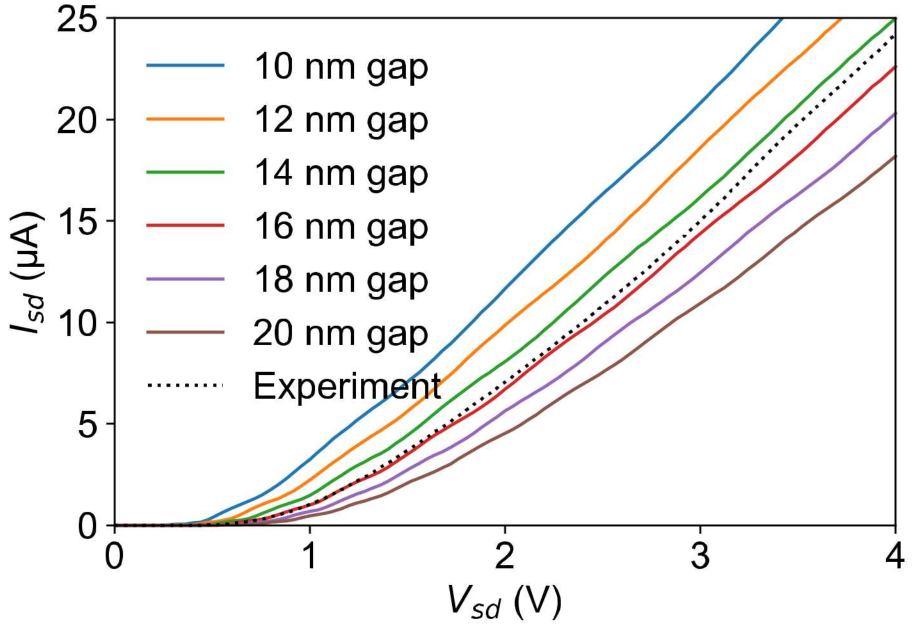
- Considered negative and positive stray charges with varying densities (in cm^{-3})
- 10 runs for each stray charge density
- Main effect: turn on voltage (similar magnitude to band structure choice)
- Some effect on variability





Conclusions

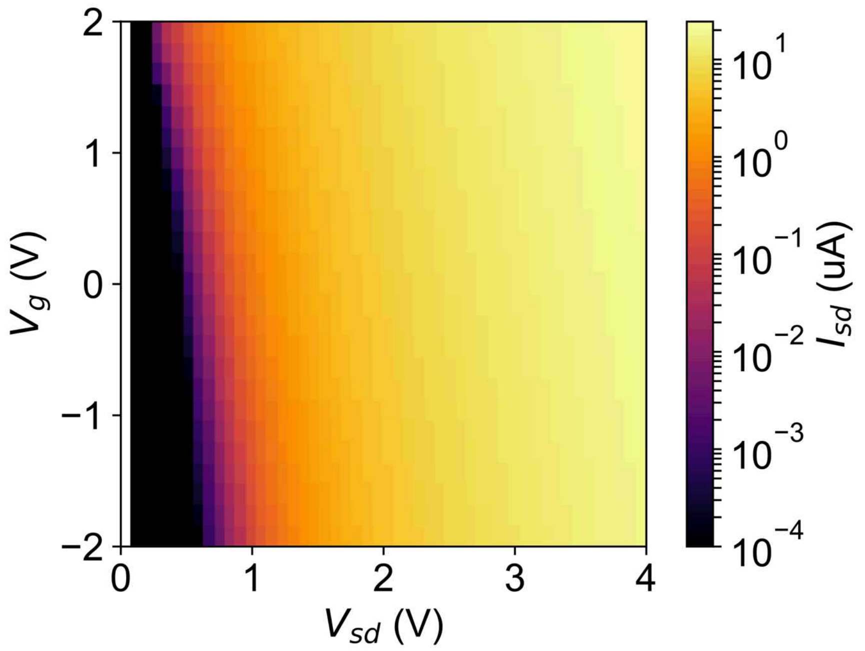
- Simple models are promising way to understand δ-doped devices
- Stray charges have effects comparable to band structure choice
- Imperfections in geometry also important
- Several good junctions could nail down the band structure



Effect of gate

- 2D model can handle more complicated devices
- Example of inplane gate
- Model predicts gate more effective than seen in experiment
- Unclear why. Reproducibility issues with our devices.

Theory



Experiment