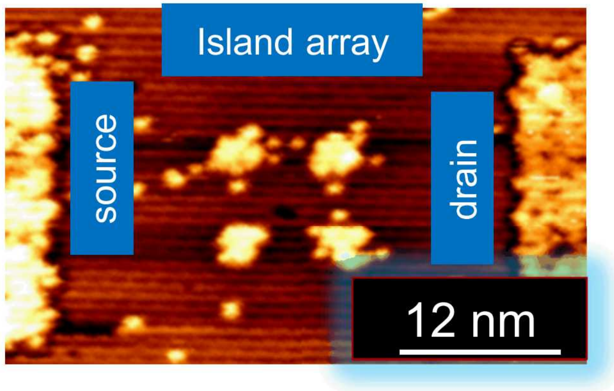
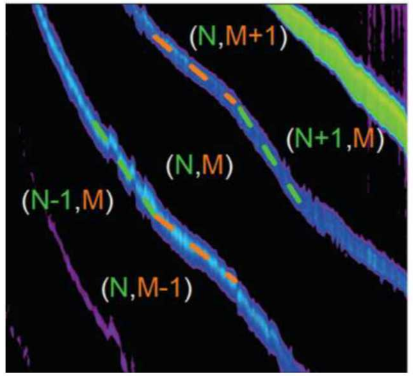
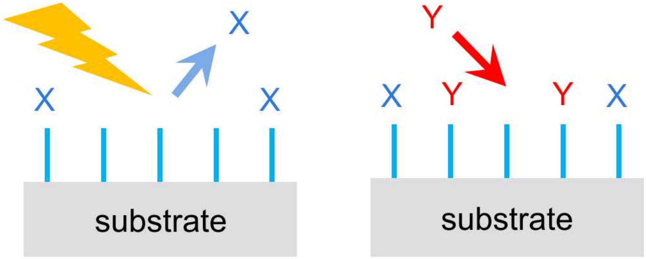
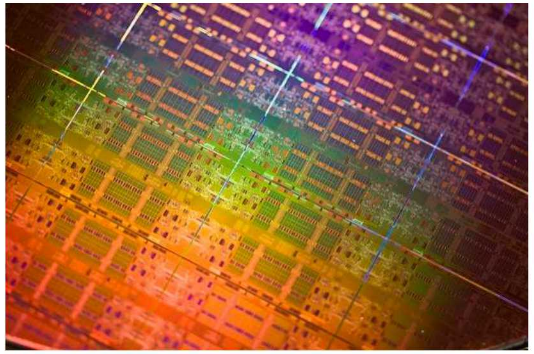
SAND2020-2755C







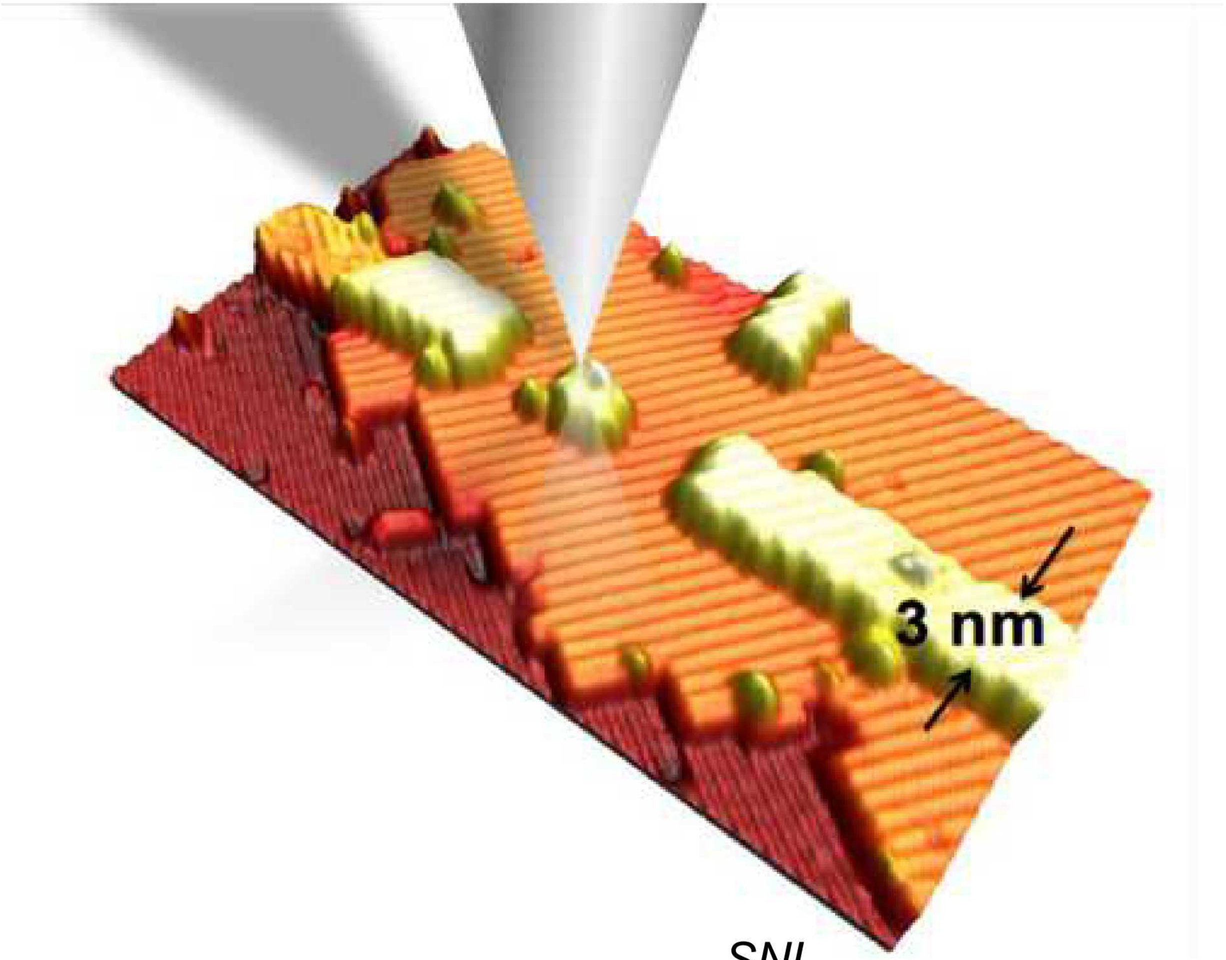


Atomic precision advanced manufacturing for electronic devices

Shashank Misra & the FAIR DEAL team

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.

Atomic **P**recision **A**dvanced **M**anufacturing



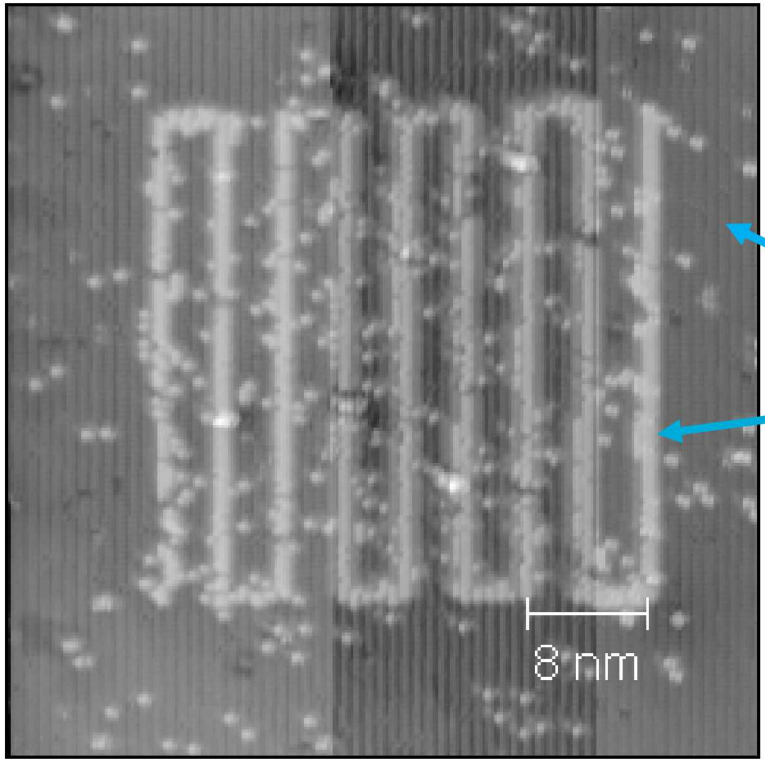
SNL

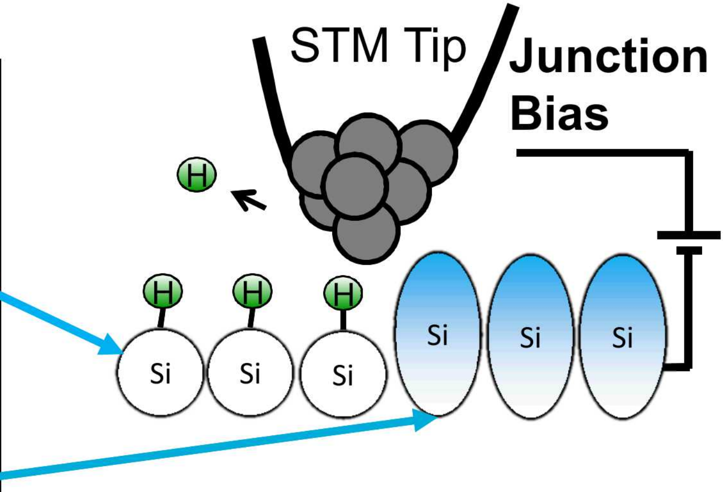
Assess the opportunities presented by atomic-scale devices and processing for the digital microelectronics of the future

How does Atomic Precision Advanced Manufacturing (APAM) work?

“Chemical contrast” at Si surface

- Unterminated Si: 1 reactive bond/ atom
- H-terminated Si: unreactive

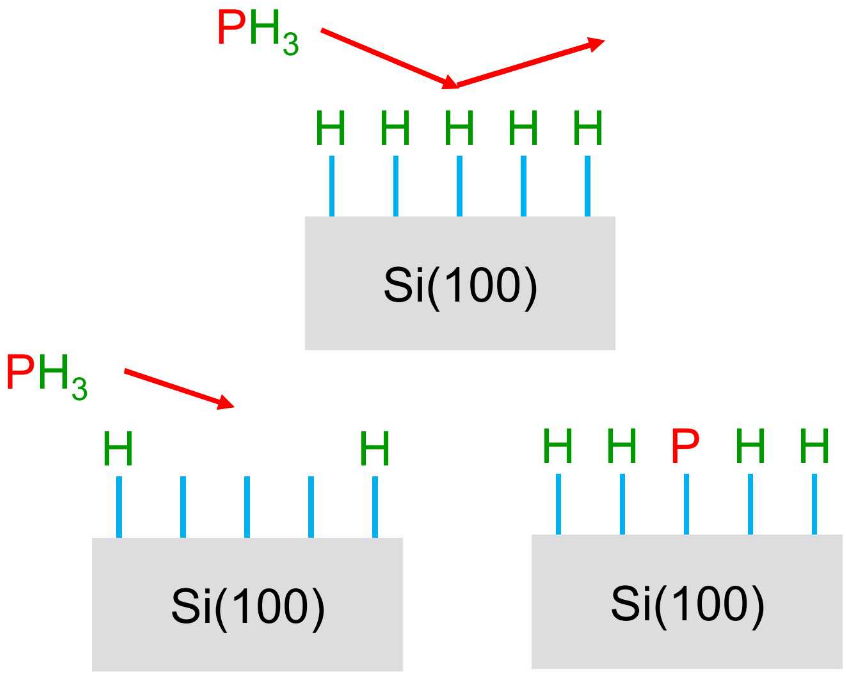




Scanning tunneling microscope (STM) can image and pattern the surface

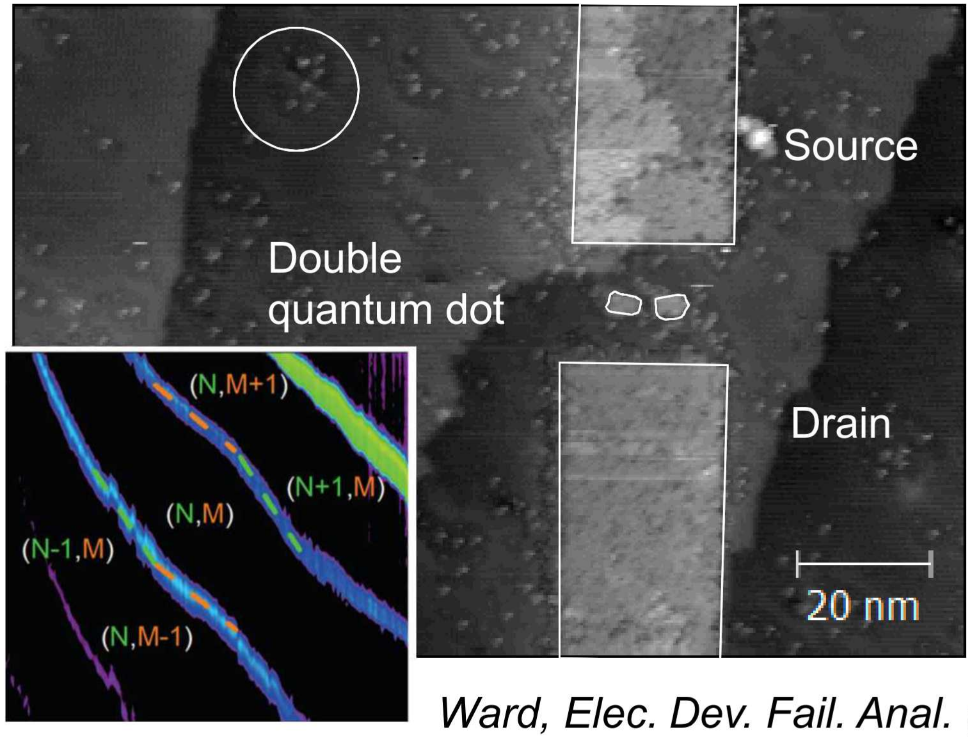
Opportunity #1: atomic-scale dopant placement

Phosphorus ‘donates’ an electron to silicon.



Chemical error correction : need 3 open sites for phosphine

Top view

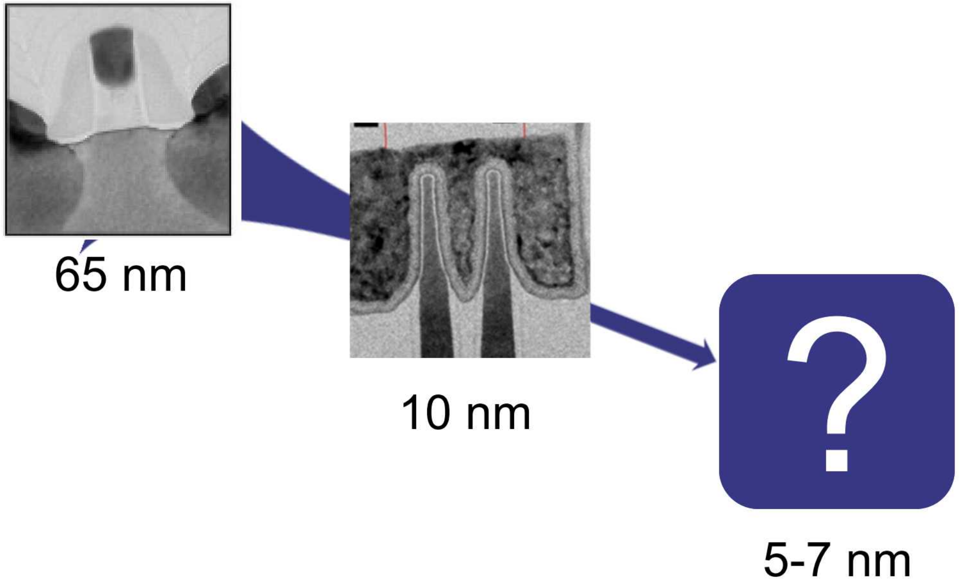


Ward, Elec. Dev. Fail. Anal. (2020)

Opportunities outside of just atomic-scale devices for quantum demonstrations

Guiding long-term goals

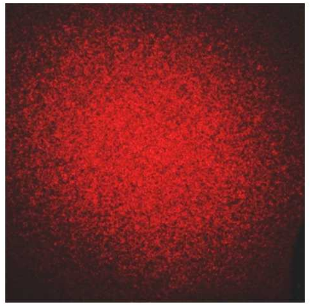
Rising cost to R&D and unclear technology path



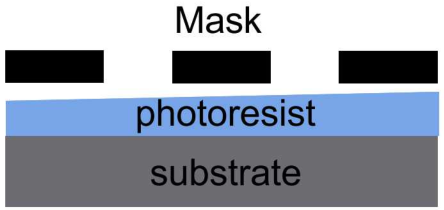
Assess device ideas from **the atomic limit**

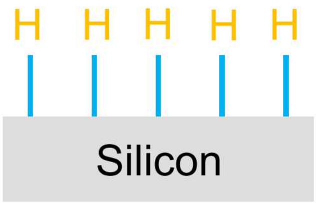
Increasing difficulty from process limitations

Inhomogeneity of light



Inhomogeneity of resist

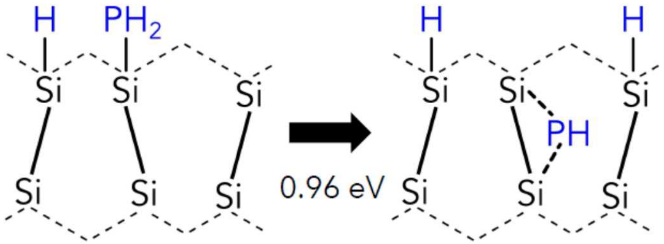




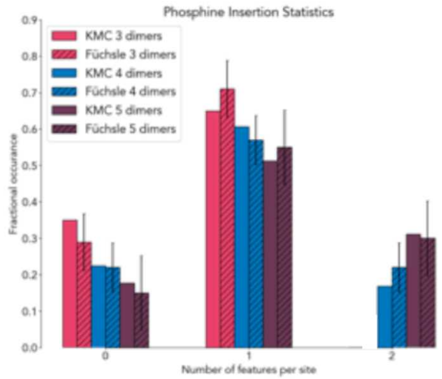
New processing paradigm with **atomic-scale chemistry**

Katzenmeyer, SPIE (2020)

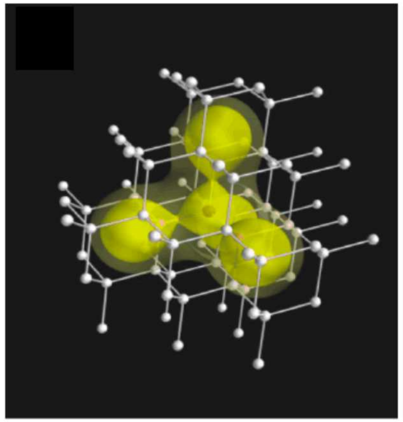
Quinn Campbell, R63.00006, Thursday 9:24, Ballroom 4D
Modeling the Electronic Structure of Phosphorus Donor Clusters in Quantum Devices



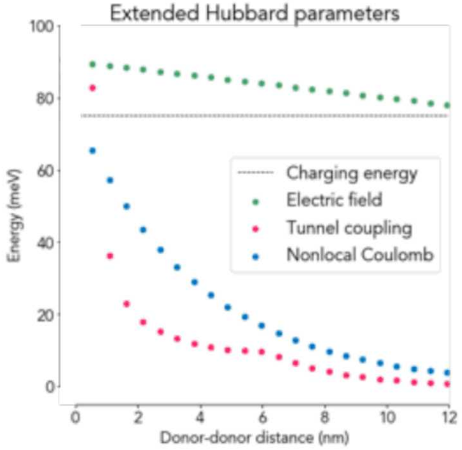
Density Functional Theory



Kinetic Monte Carlo



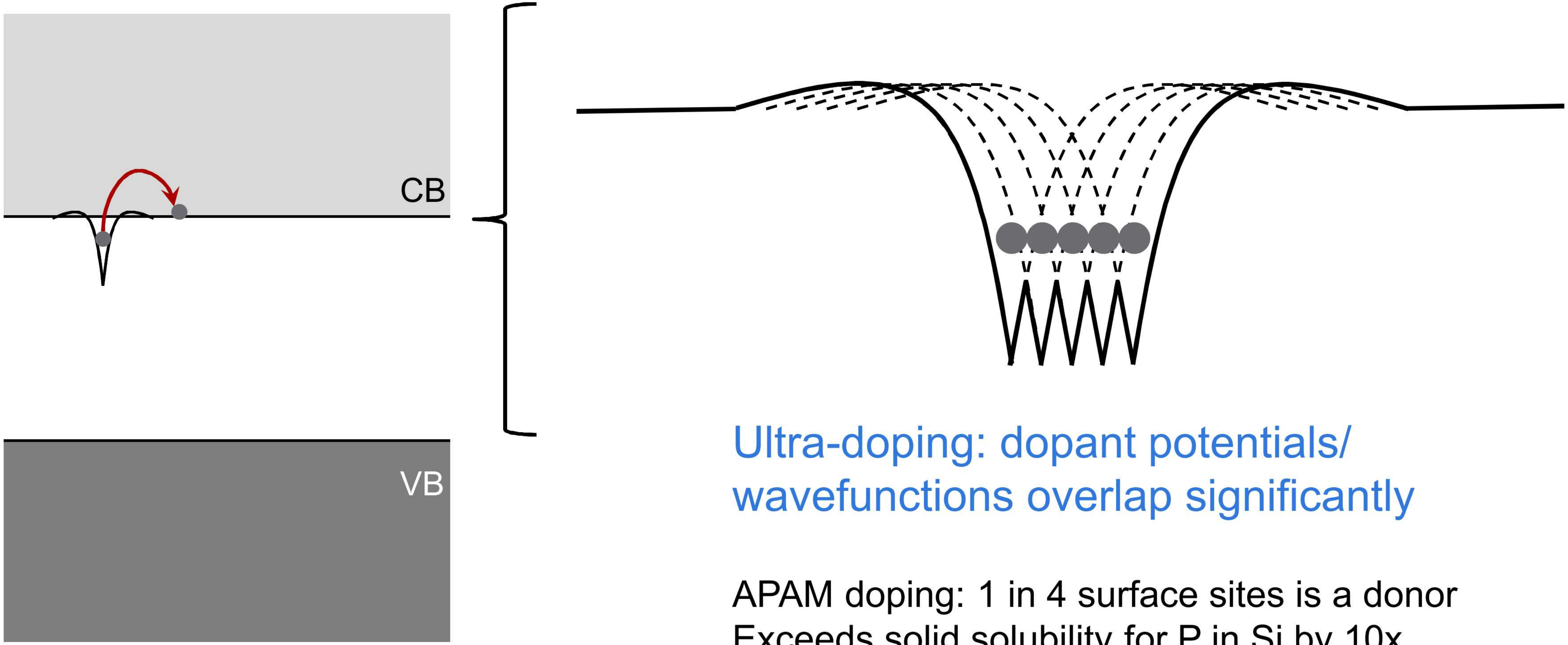
Effective Mass Theory



Electronic Property Modeling

Phosphine incorporation is non deterministic, modeling allows us to predict electronic consequences

Opportunity #2: “Ultra-doping”

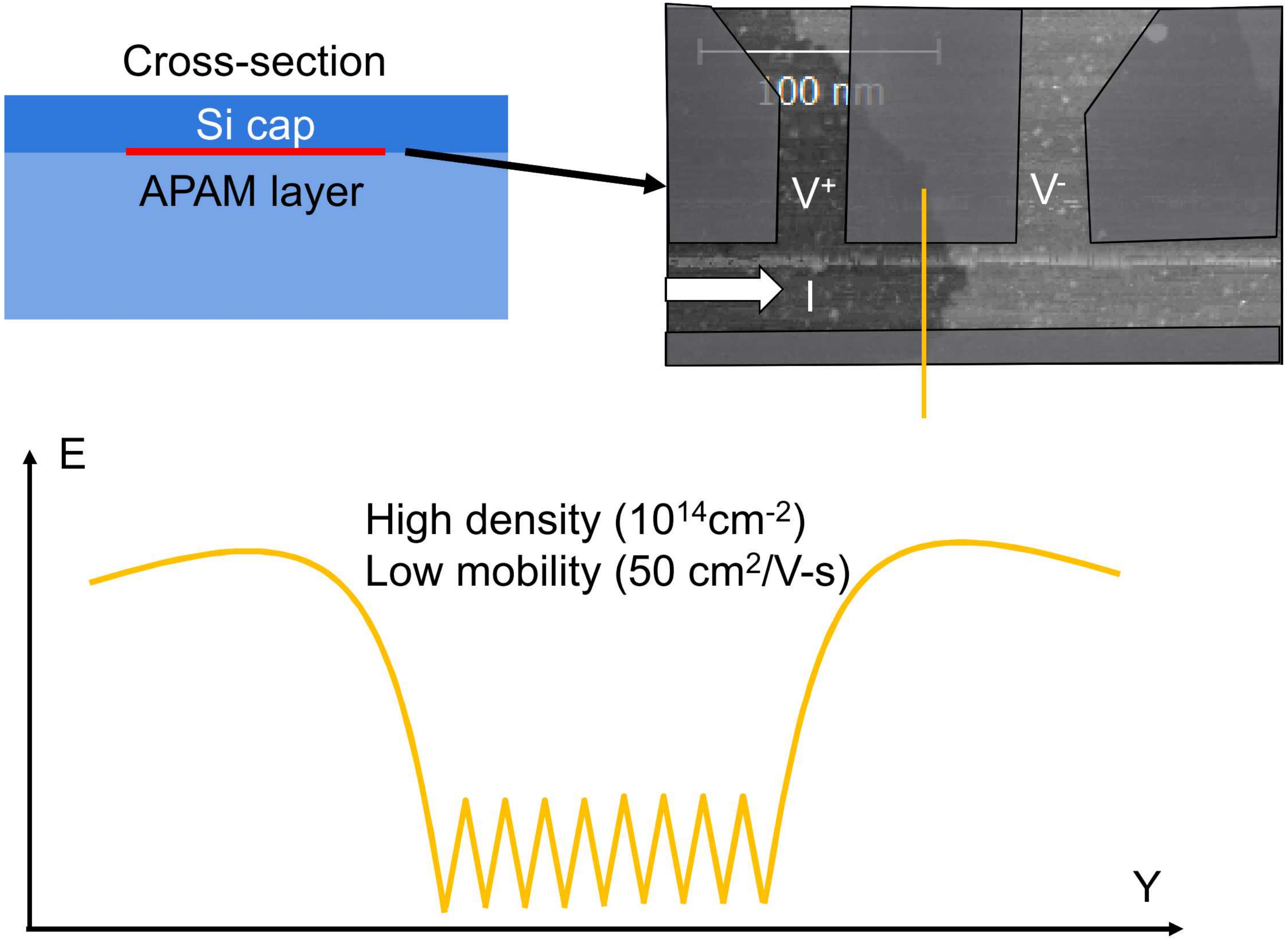


Normal doping

Ultra-doping: dopant potentials/ wavefunctions overlap significantly

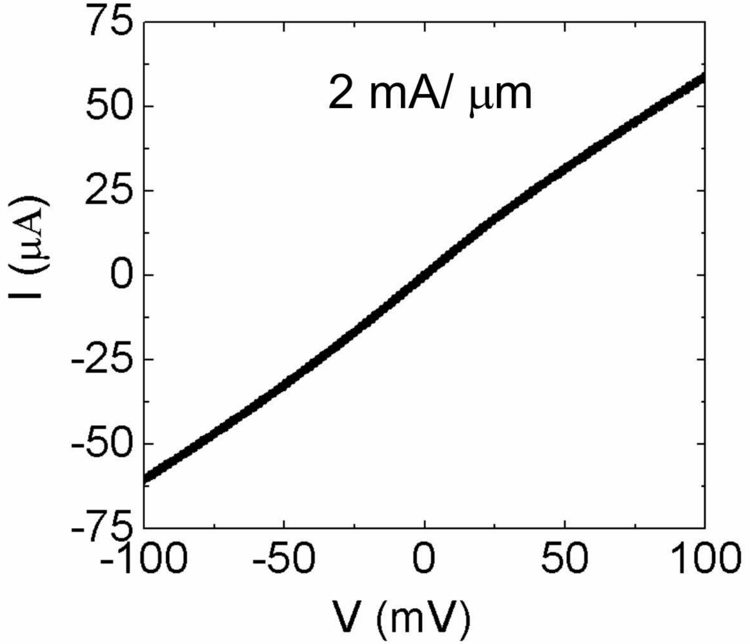
APAM doping: 1 in 4 surface sites is a donor
Exceeds solid solubility for P in Si by 10x

Consequences: confinement



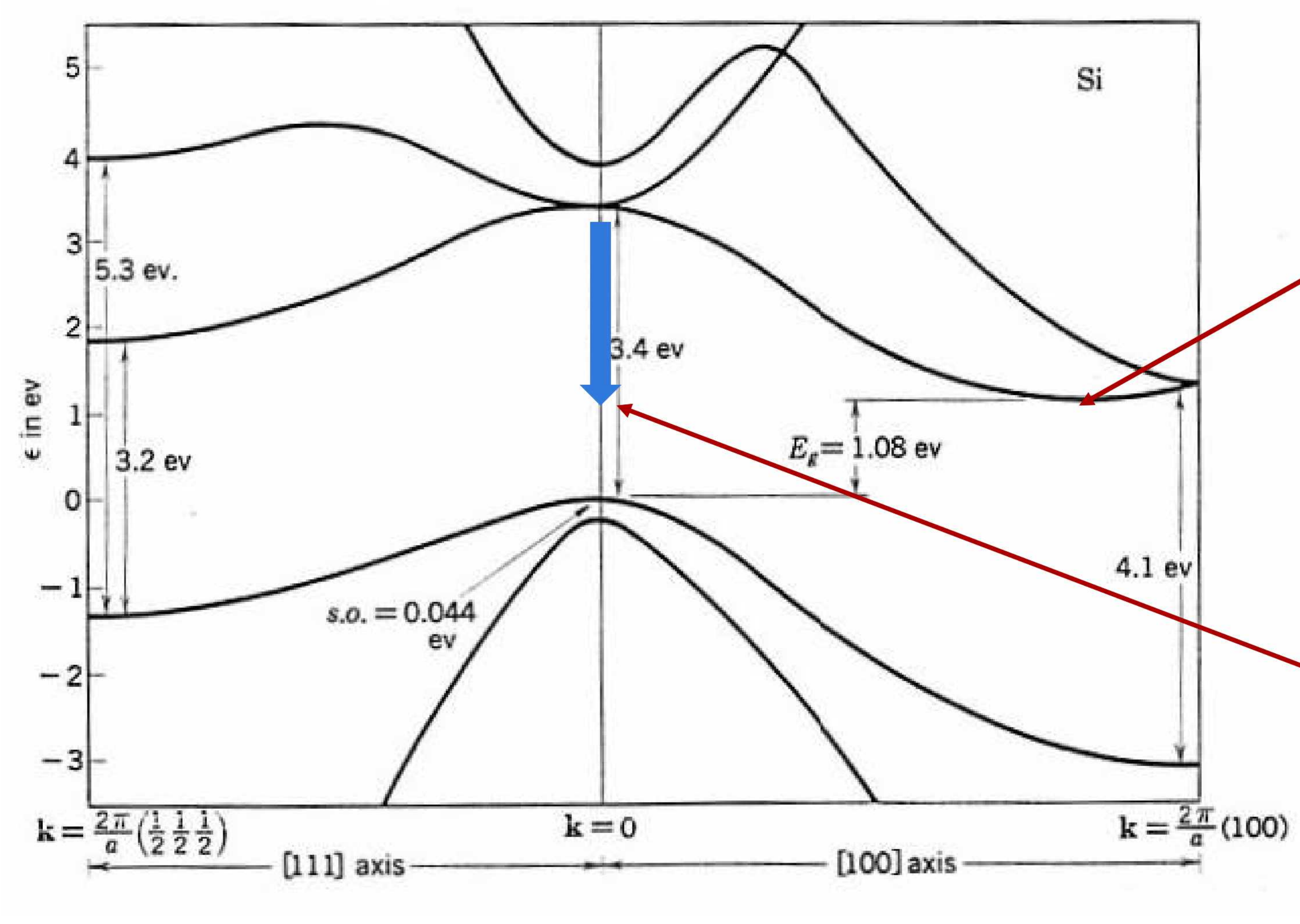
High density (10^{14}cm^{-2})
Low mobility (50 cm^2/V-s)

Ward, Elec. Dev. Fail. Anal. (2020)

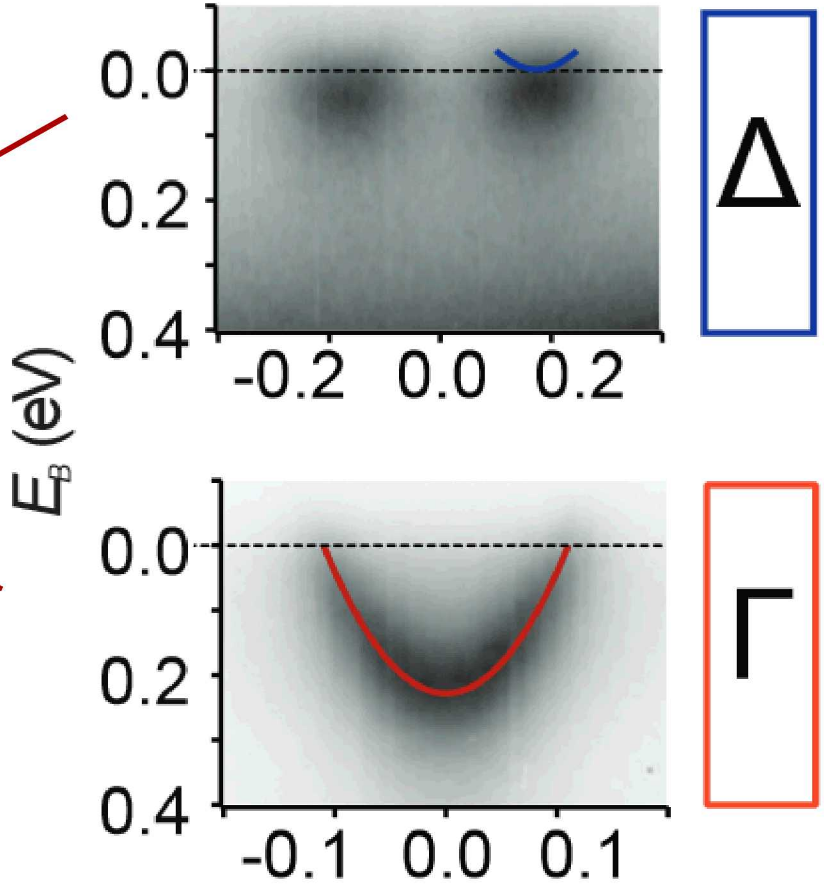


Dopants give you confinement
Extremely high current density.

Consequences: electronic structure

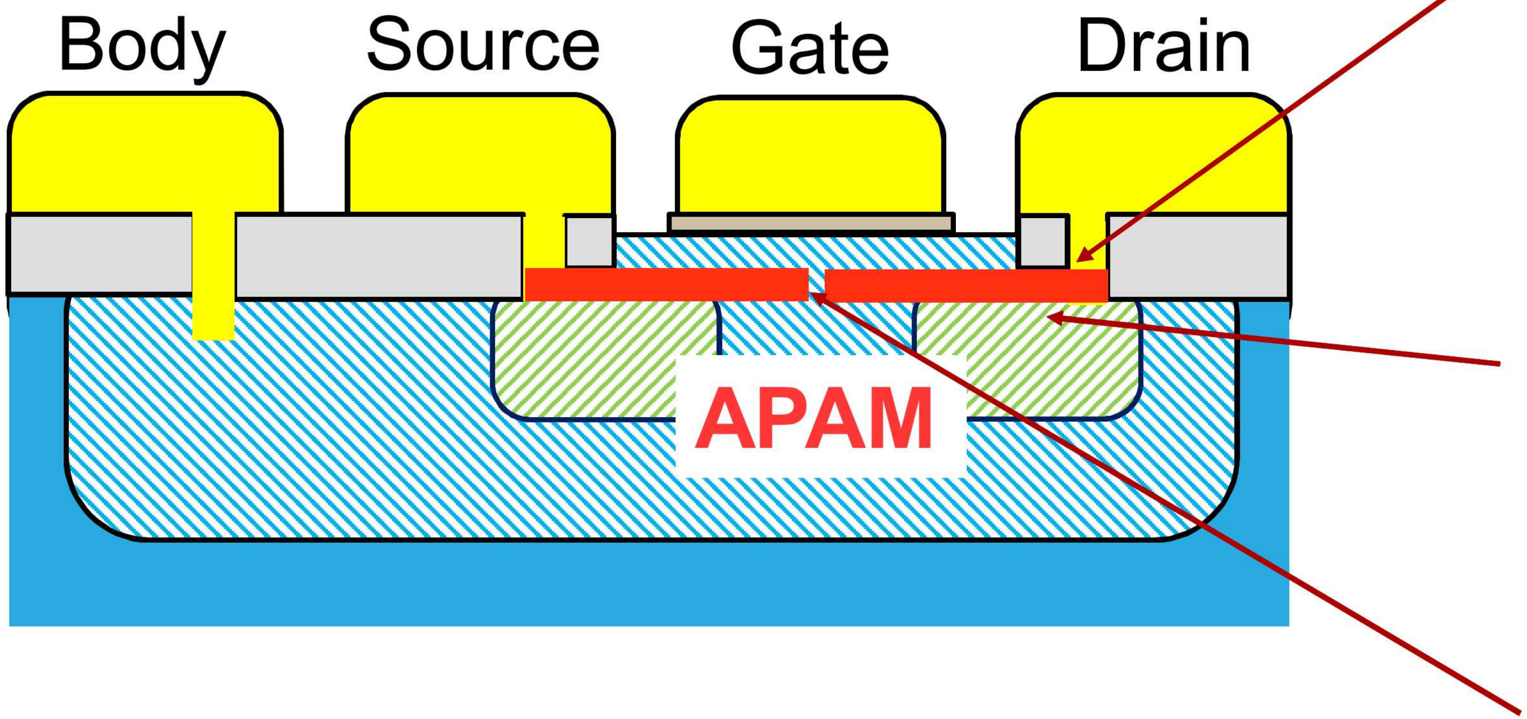


This isn't really silicon like you know it.



Holt, arXiv:1911.08274

APAM-inspired transistor



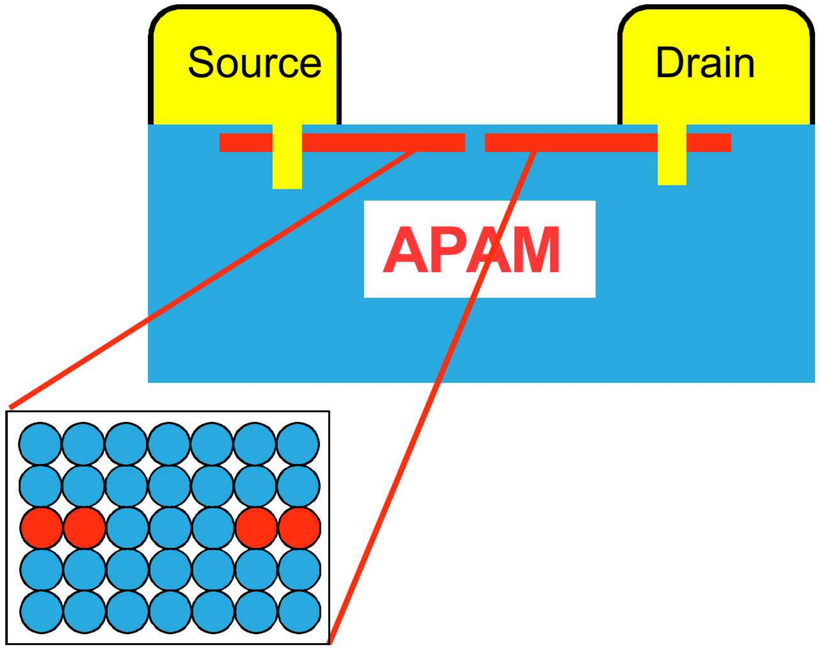
Schottky barrier manipulation
Low contact resistance

Confinement
High current density

Band-to-band tunneling
Low voltage operation

What’s missing (outline)?

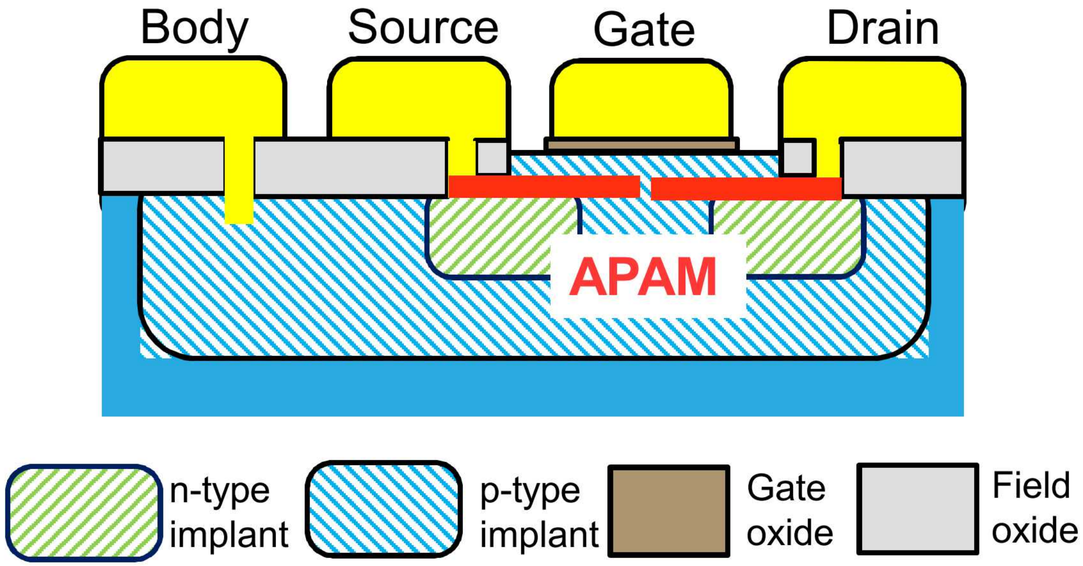
Now (3 US labs, 6 labs worldwide)



- Only works at cryogenic temperatures
- Gates are in-plane
- Phosphorus only

Desired future state

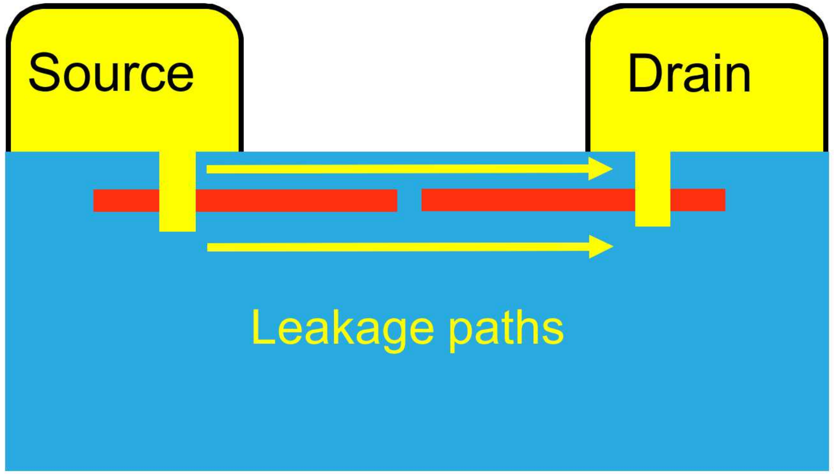
“Real” transistor

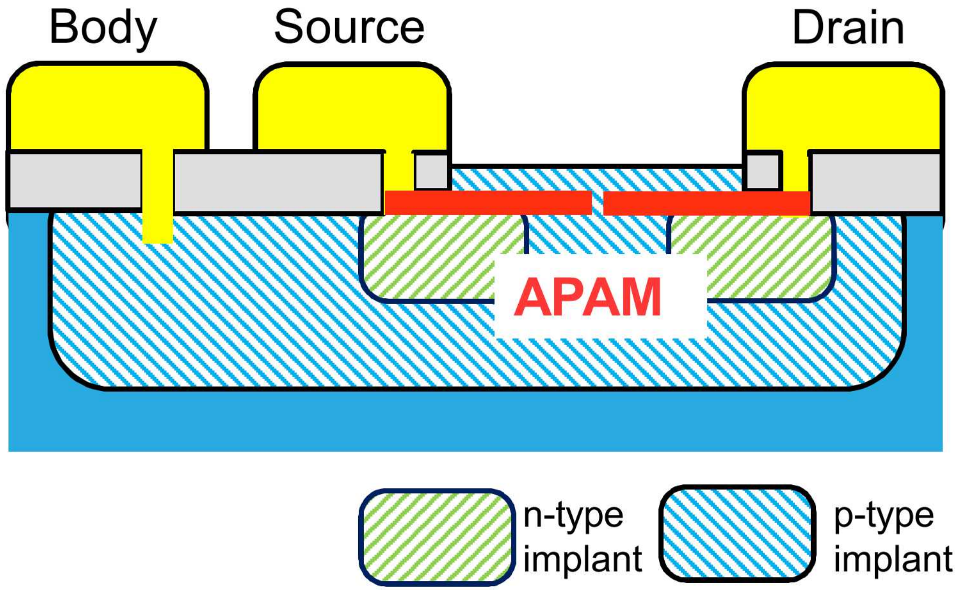


1. **Works at room temperature**
2. **High-gain surface gate**
3. **Complementary transistors**

1. Room temperature operation

Cryogenic temperatures freeze leakage paths



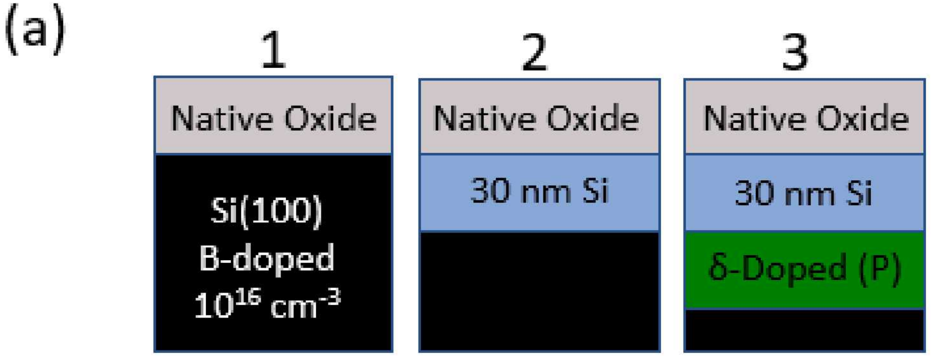


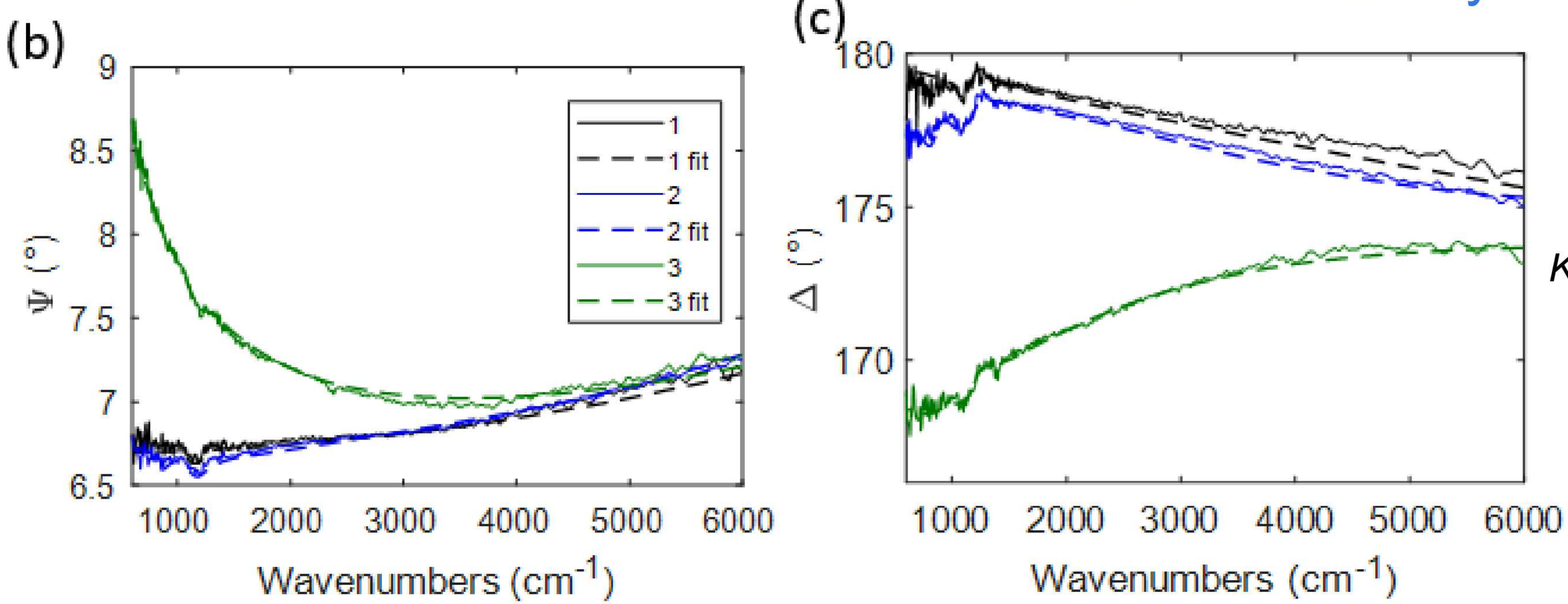
Adopt CMOS doping schemes to limit leakage for room temperature operation

Do ultra-doped layer work at room temperature?

Yes! See Drude response of a dense 2D sheet of electrons at room temperature.

Mobility about same at 293K, 4K
Carrier density about same at 293K, 4K

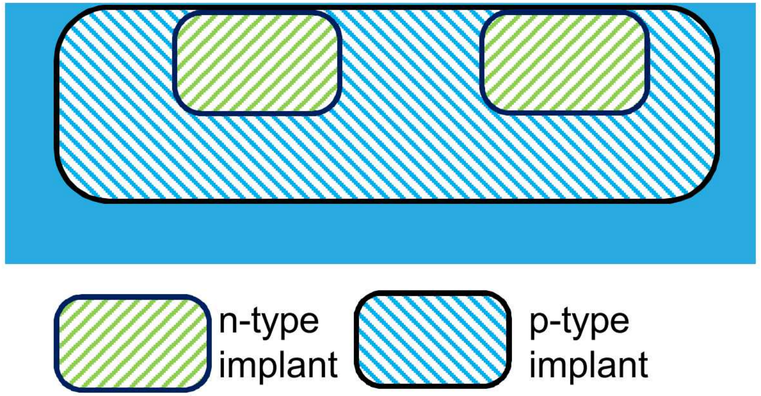




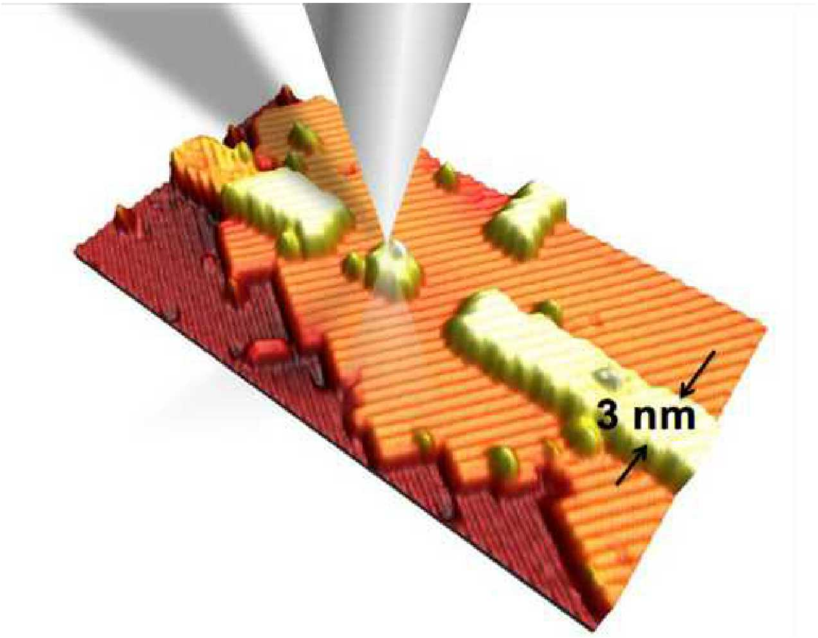
Katzenmeyer, arXiv 2002.xxxxx

Can we control leakage paths?

Starting material



APAM 1200°C Process

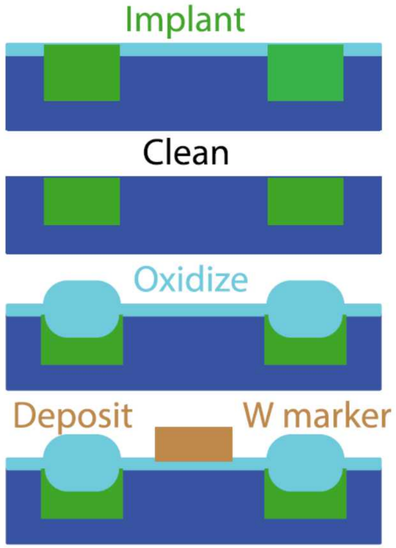


Typical APAM sample clean: Joule heat chip to 1200° C.

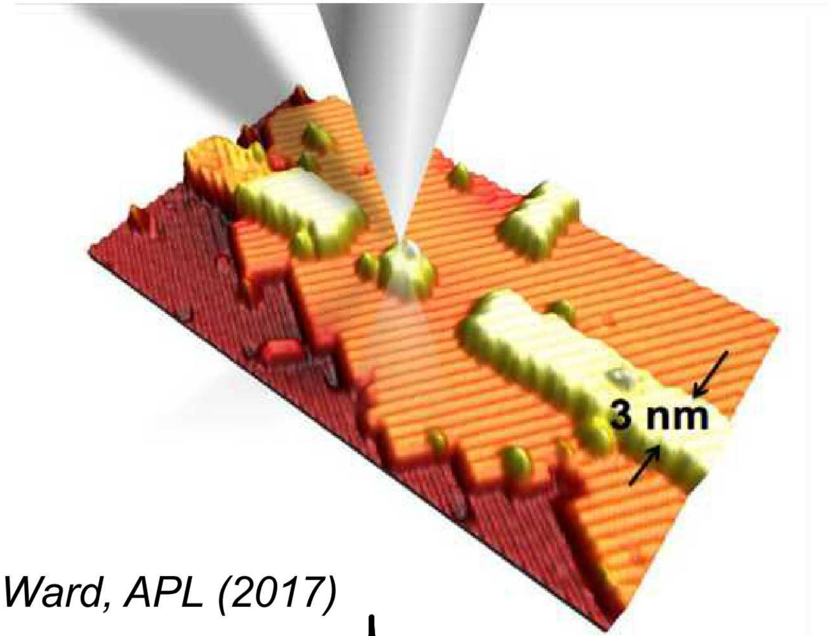
Phenomenal surface, but will not preserve dopant profiles

Reduced temperature processing

High T Processes (>850°C)

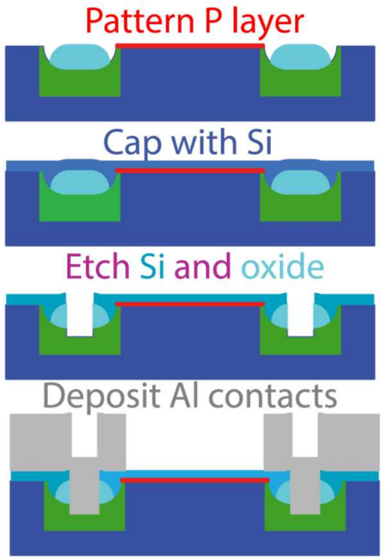


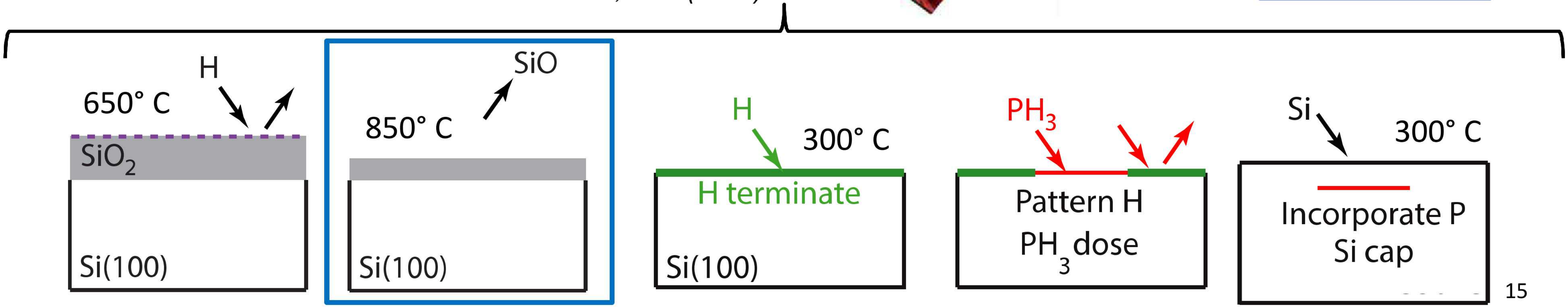
APAM 850°C Process



Ward, APL (2017)

<450°C Processes





More to it than just thermal budget

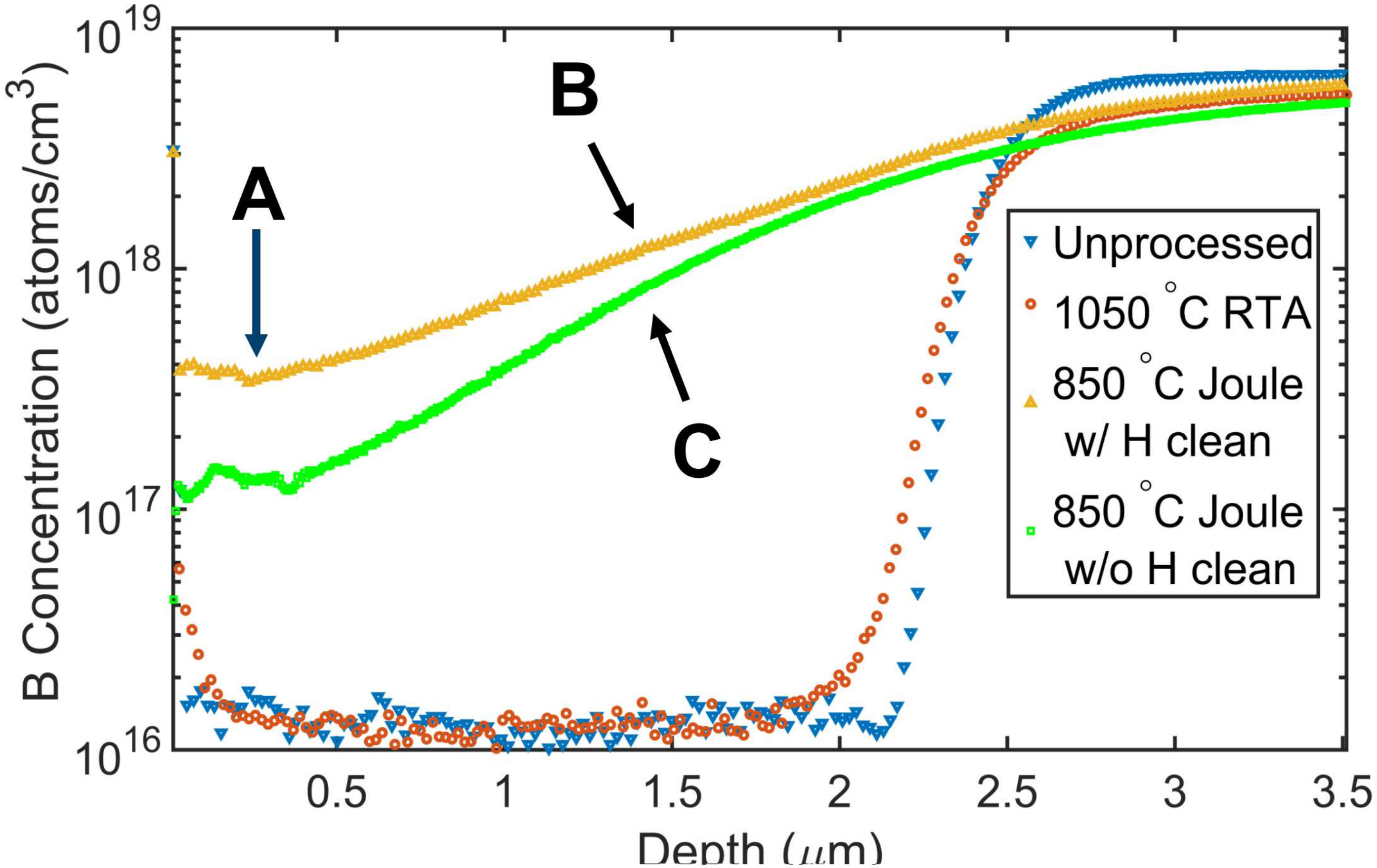
Si (100) chip under test

p-	B: ~1x10^{16} atoms/cm^3
p++	B: ~8x10^{18} atoms/cm^3

Understand A (chamber) and B (hydrogen)

Joule heating appears to cause C

Need new method to prepare chips!



Jeff Ivie, P63.00007, Wed. 4:06, Ballroom 4D

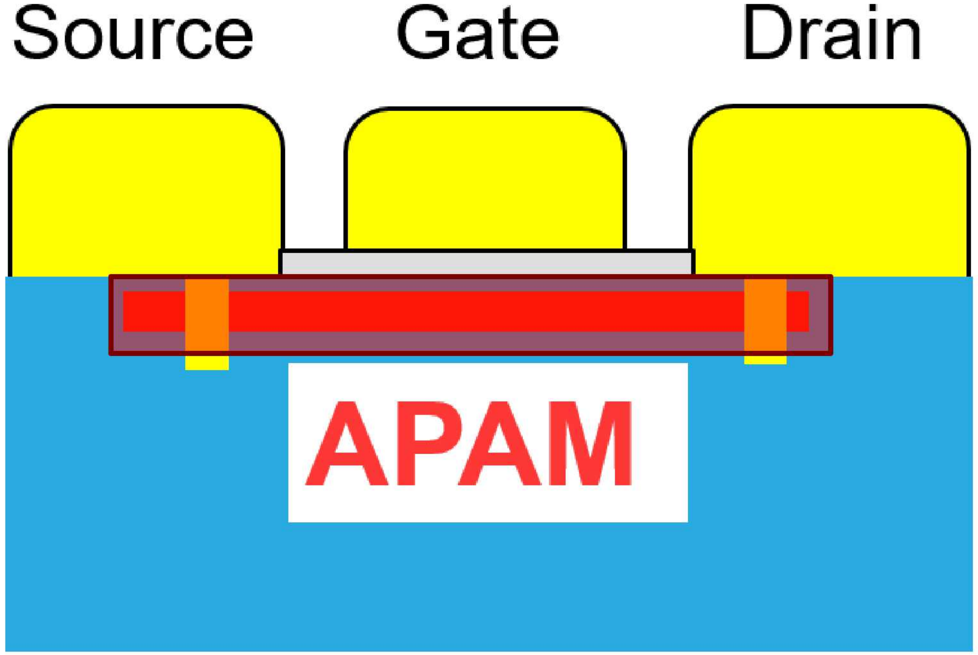
Diffusion of Acceptor Dopants in Atomically Precise Devices

2. Surface gates

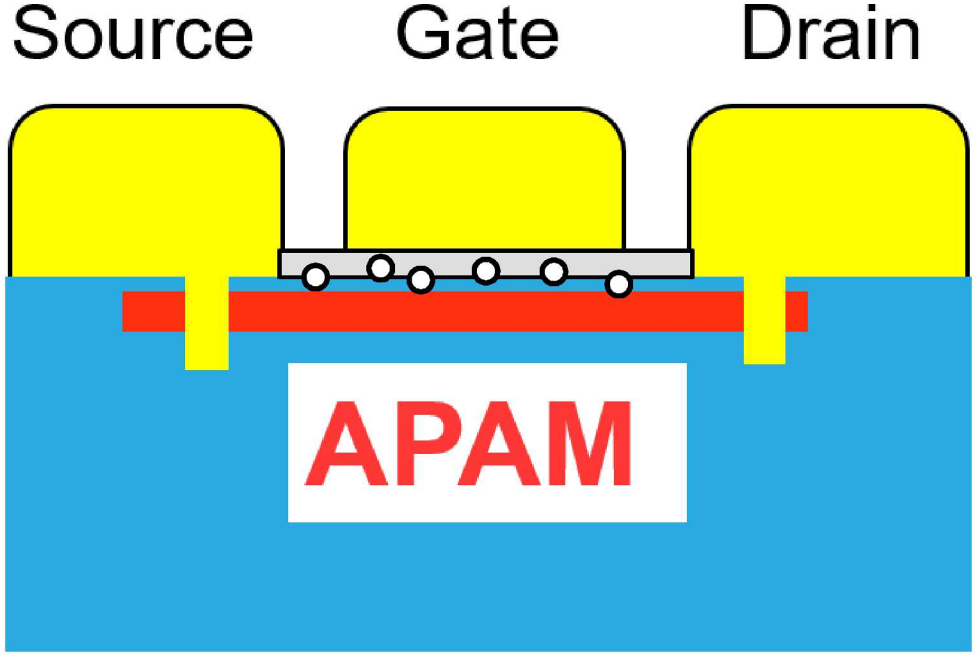
In-plane dopant-based gates inadequate for transistor applications

Different thermal compatibility issue for surface gates: keep dopants in place

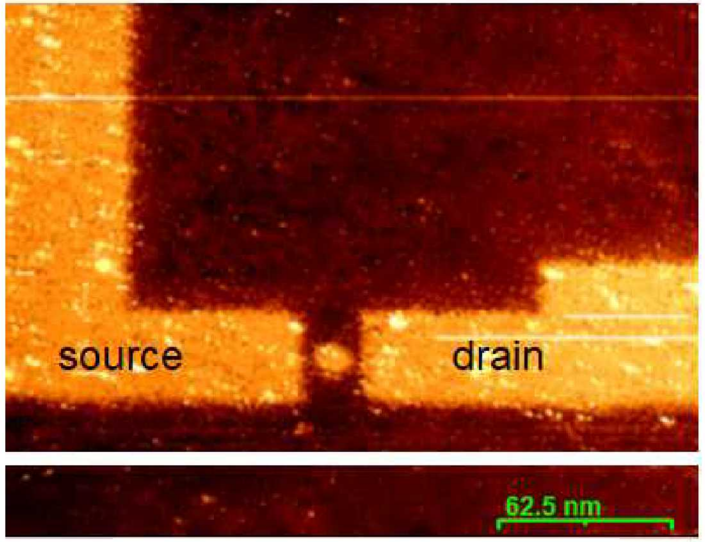
High-temperature processing destroys APAM devices

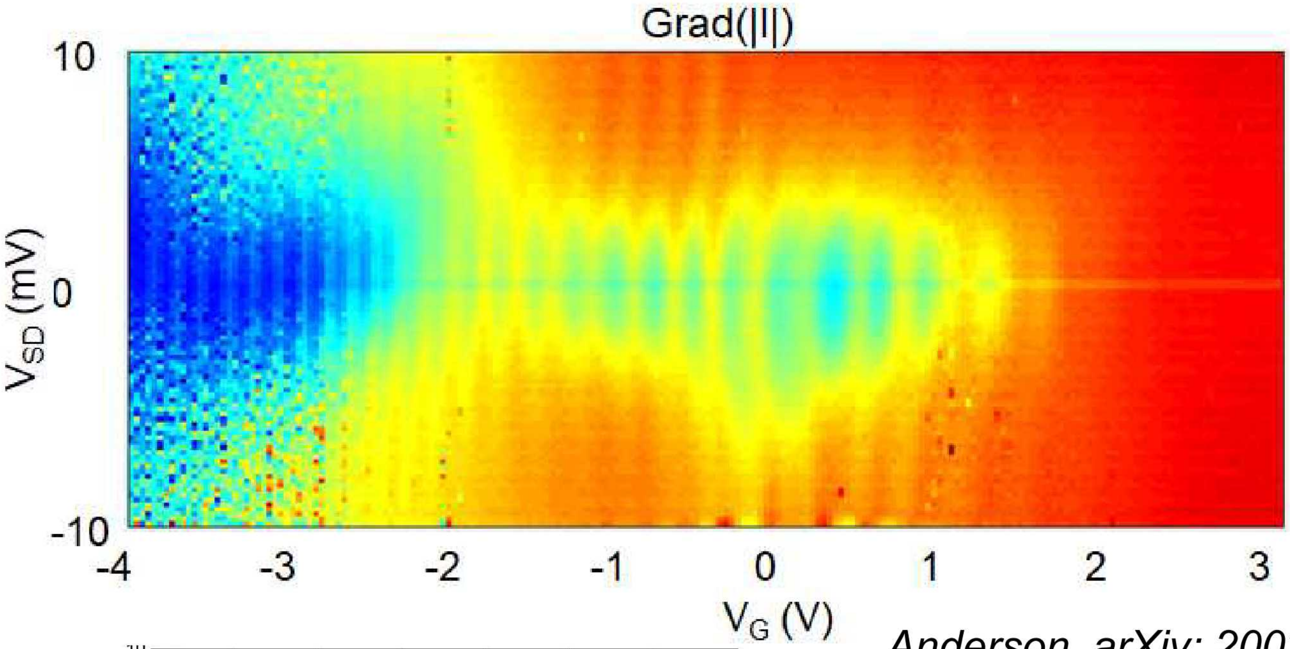


Low temperature gate stack could be defective

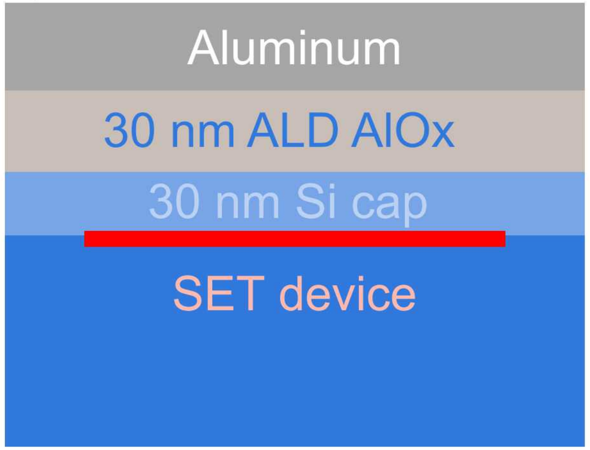


Top-gated single-electron transistor





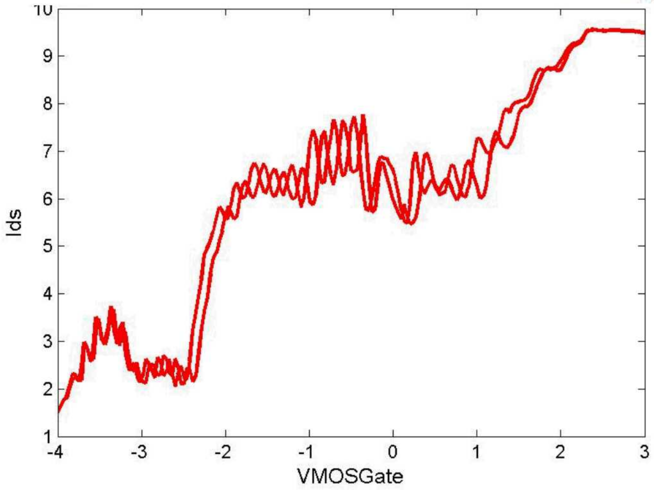
Anderson, arXiv: 2002.09075


Aluminum

30 nm ALD AlOx

30 nm Si cap

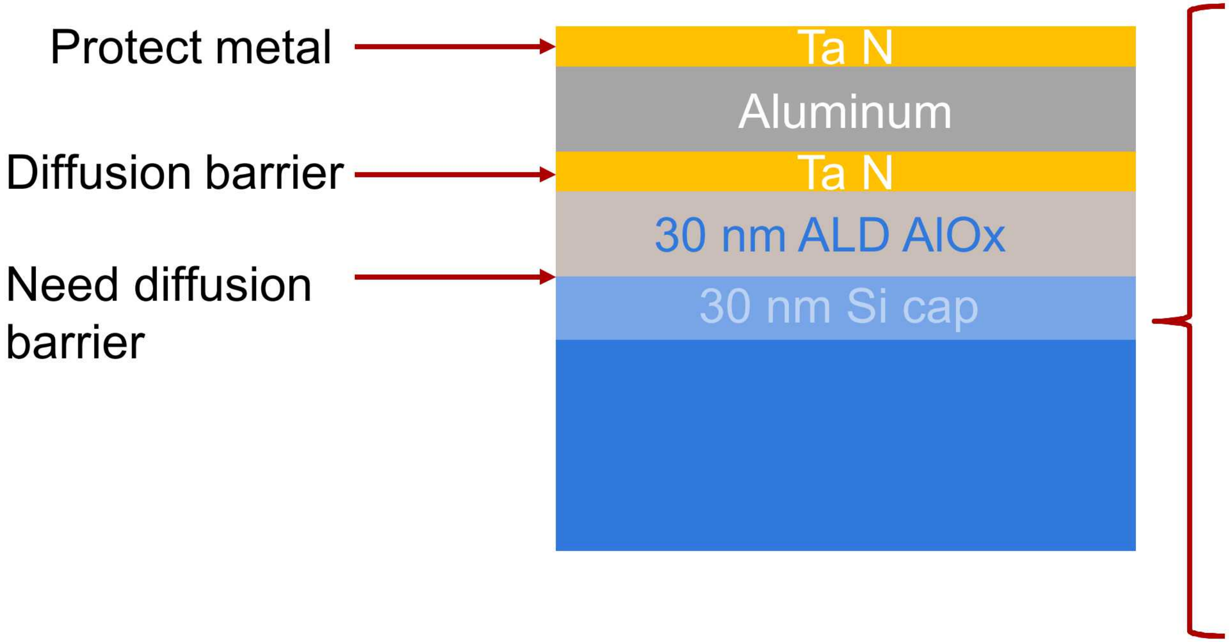
SET device



The gate works.
Improvement required.

New gate stack

To keep the APAM layer intact, the process flow has a low thermal budget.



Protect metal

Diffusion barrier

Need diffusion barrier

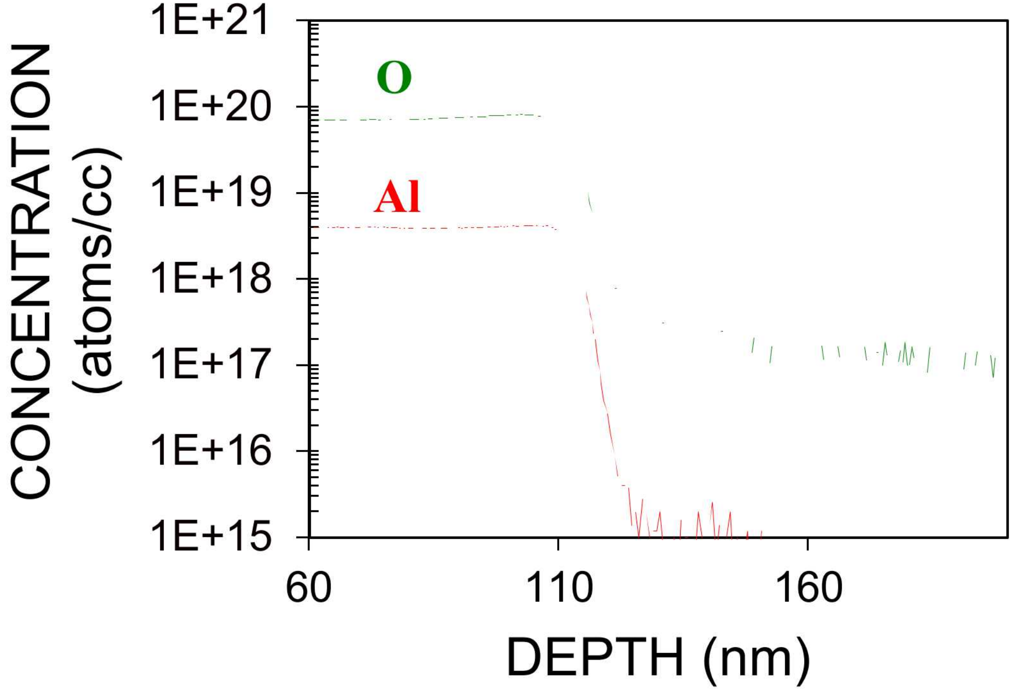
Ta N

Aluminum

Ta N

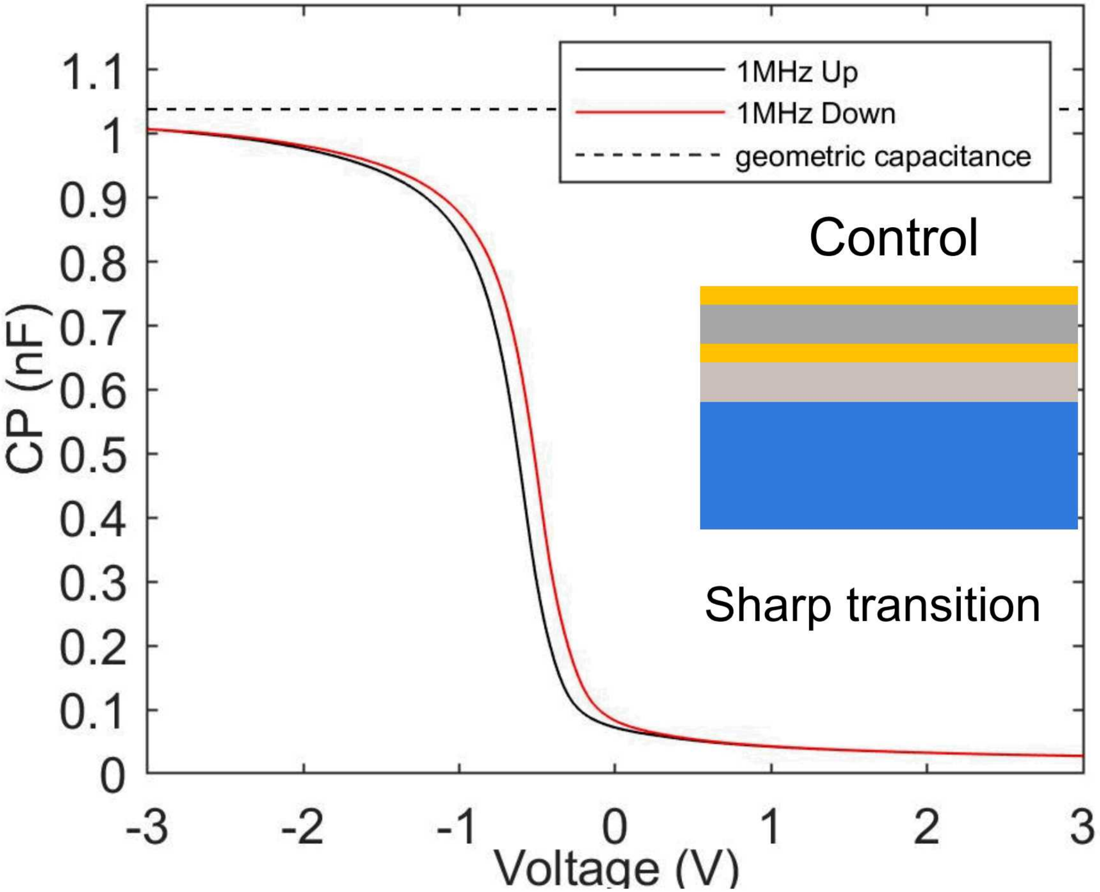
30 nm ALD AlOx

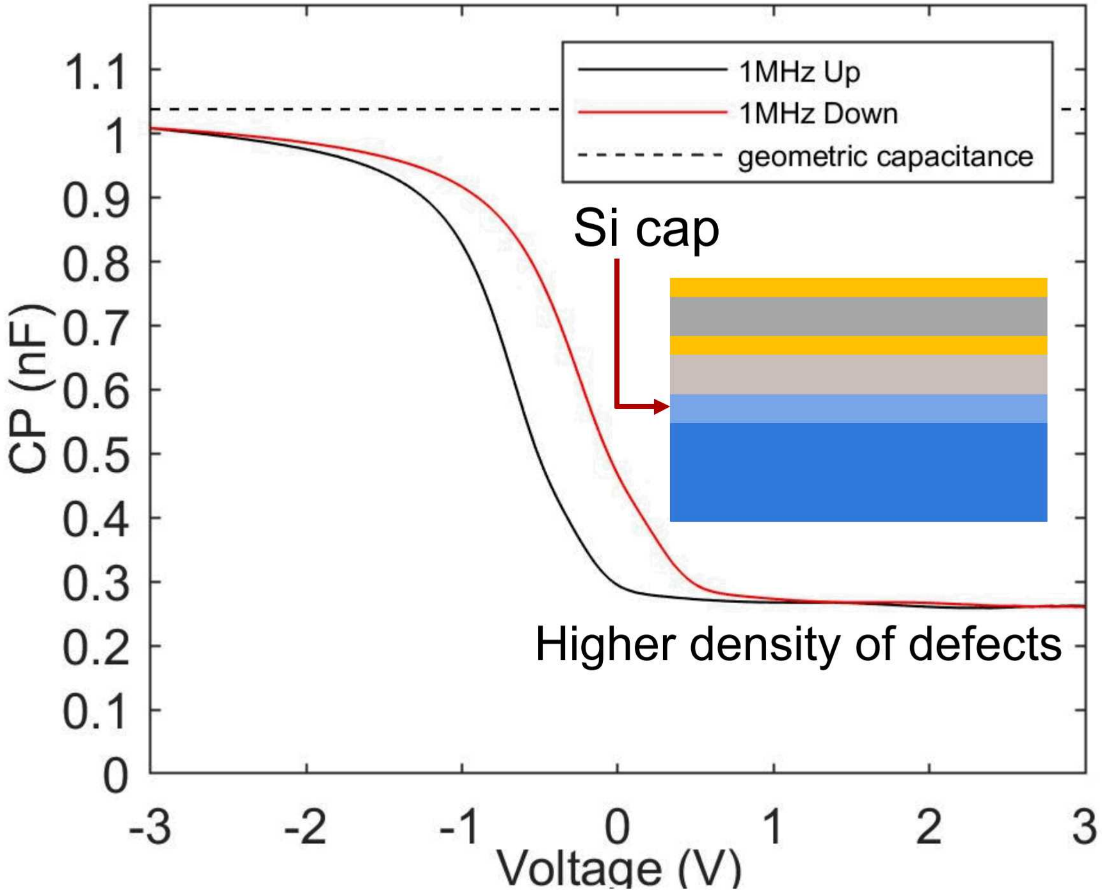
30 nm Si cap


Composition of sublimation source Si caps

New gate stack – MOS capacitors

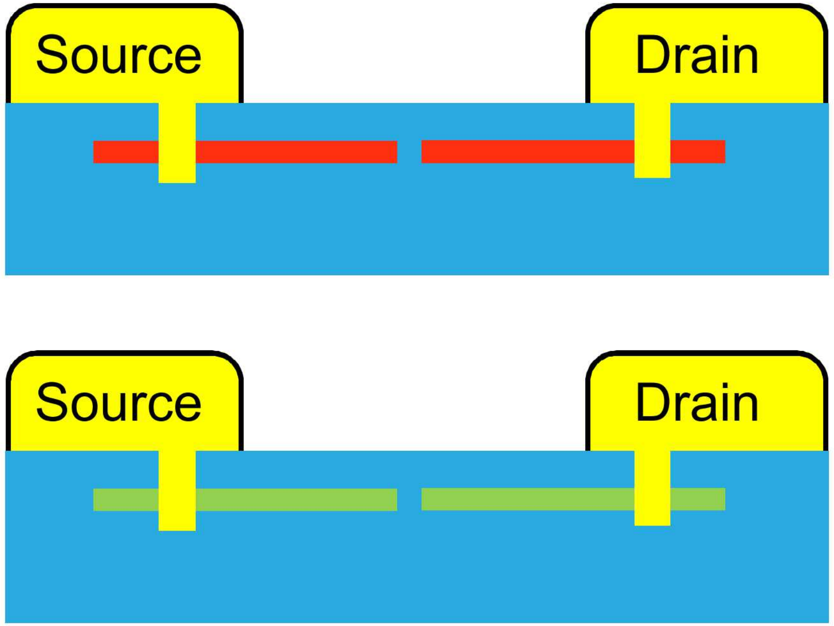
Even a low-temperature oxide is of higher quality than APAM ‘epitaxial’ silicon.

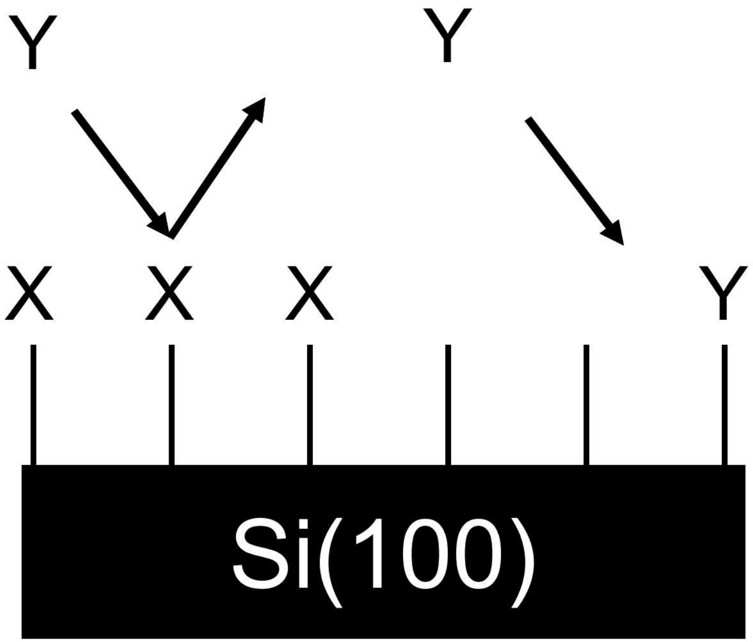




Tzu-Ming Lu, D27.00001, Mon. 2:30, 404
Development of a high-k gate stack for atomic-precision advanced manufacturing

3. Complementary transistors





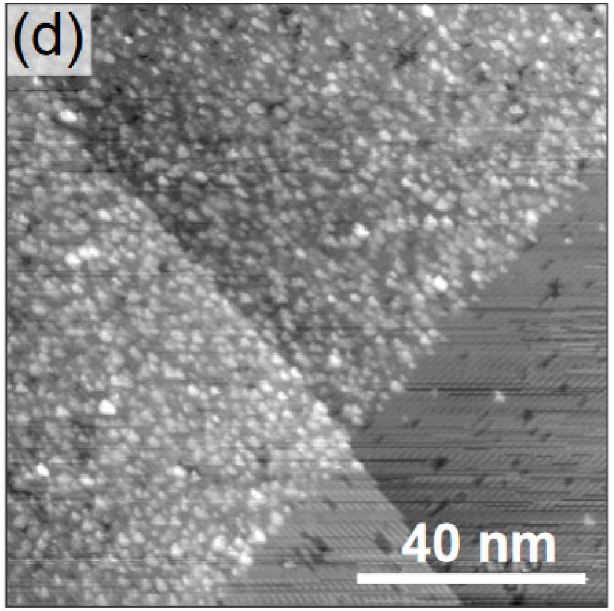
Need complementary carrier – atomic precision, ultra-dense holes!

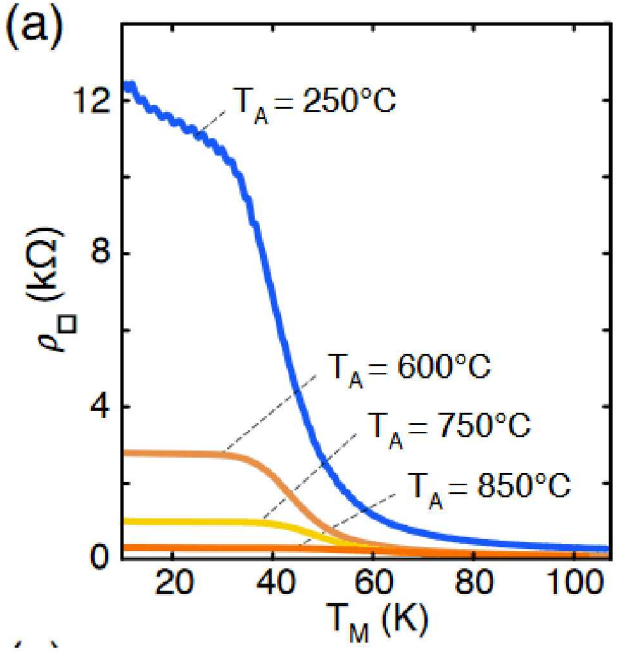
Requires

- Selective to atomic resist (X = hydrogen or halogen)
- Incorporation while X remains intact
- Ultra-high density of active incorporation

Diborane provides selective p-type doping

Skeren, arXiv:1912.06188





B_2H_6 sticks selectively!

Electrical quality is questionable at temperatures where hydrogen resist survives.

Current approach: guess and check (and pray…)

Requires

- Selective to atomic resist (X = hydrogen or halogen)
- Incorporation while X remains intact
- Ultra-high density of active incorporation
- **Time!!!!!! Takes a year to try anything.**

Acceptor	Hydride	Halide	Organic
Boron	B_2H_6 $B_{10}H_{14}$	BCl_3 BF_3 BBr_3	Trimethylboron
Aluminum	AlH_3	$AlCl_3$	Trimethylaluminum Triethylaluminum
Gallium		$GaCl_3$	Triethylgallium
…	…	…	…

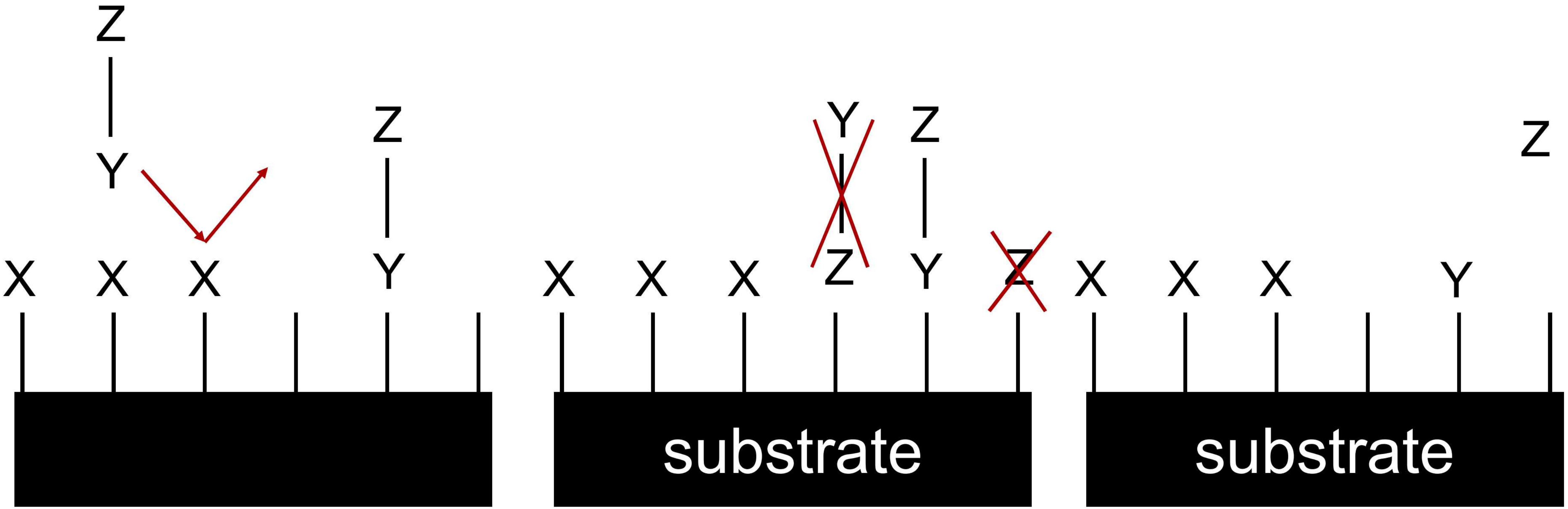
What happens when I need an atomic precision gate?

Requirements are stiff. Need new approach.

- Selective
- Self-limited

- Clean, direct attachment

- Can remove ligands
- Error-correcting



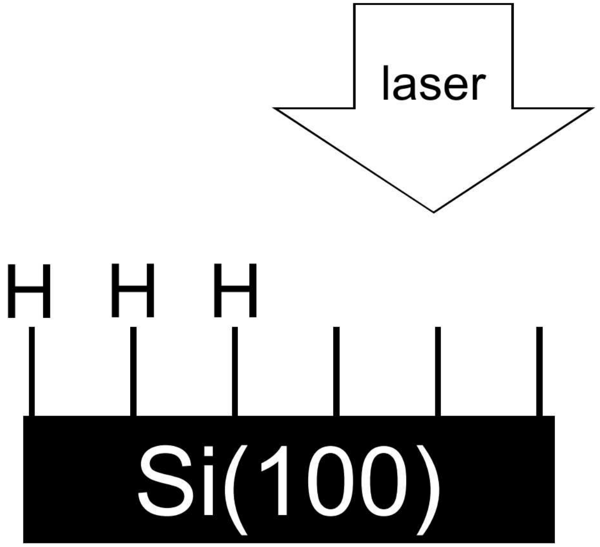
1. Model precursors for selective attachment

2. Synthesize molecules

3. Modify molecules once on surface

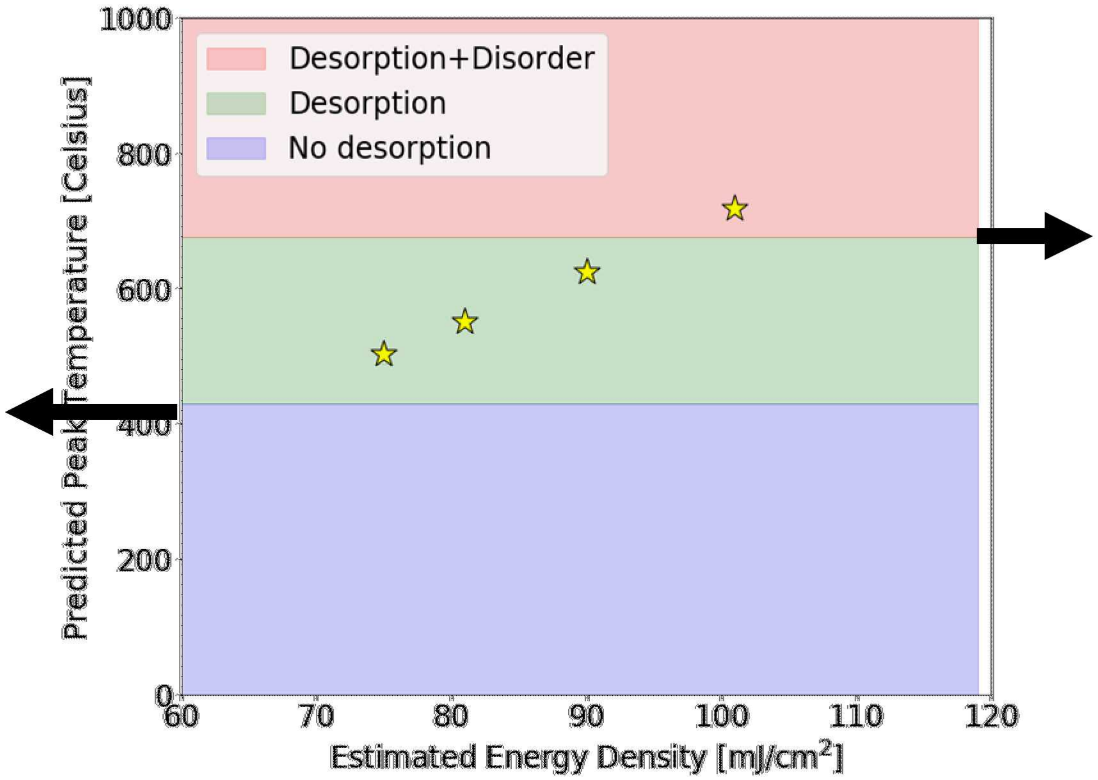
2nd step of chemistry ← likely necessary
Add energy to remove Z

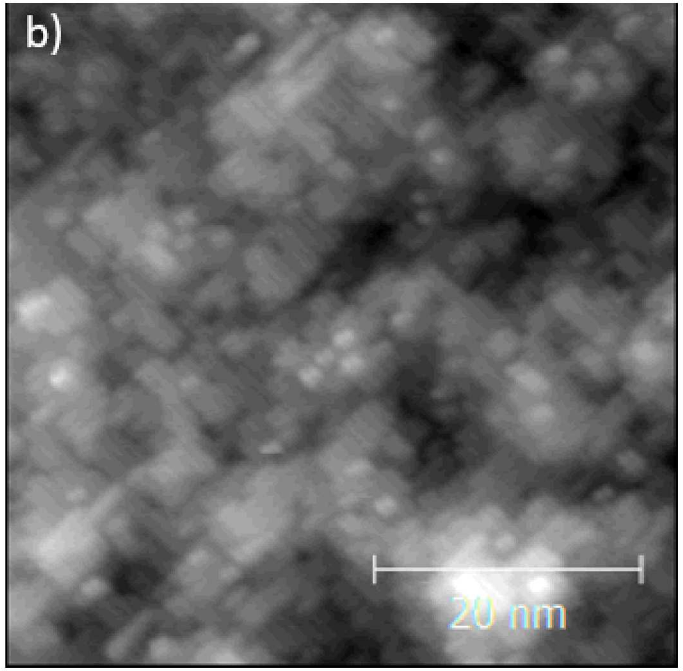
Using light to modify surface chemistry



~ 60 mJ/cm^2

Katzenmeyer, SPIE (2020)





Removing Si
~ 90 mJ/cm^2

Photothermal patterning of hydrogen.
Laser pulse duration = knob on kinetics?

Thanks to…

APAM-enabled devices
Lead: Shashank Misra

Modeling
Lead: Suzey Gao

Integration
Lead: David Scrymgeour

Scalability
Lead: George Wang

Measurement: Lisa Tracy, Tzu-Ming Lu, Albert Grine, David Scrymgeour, Ping Lu, Aaron Katzenmeyer

Microfabrication: David Scrymgeour, Andrew Leenheer, Dan Ward, DeAnna Campbell, Mark Gunter, Phillip Gamache, Sean Smith, Troy England, Andrew Starbuck, Steve Carr, Reza Arghavani

Modeling: Suzey Gao, Denis Mamaluy, Juan P. Mendez, William Lepkowski, Michael Goldflam, Amun Jarzembski, Thomas Beechem, Andrew Baczewski, Quinn Campbell, Steve Young, Peter Schultz

Surface Science: Ezra Bussmann, Scott Schmucker, Evan Anderson, Joe Lucero, Jeff Ivie, Fabian Pena, Aaron Katzenmeyer, George Wang, Esther Frederick, Igor Kolesnichenko, David Wheeler, Mike Marshall

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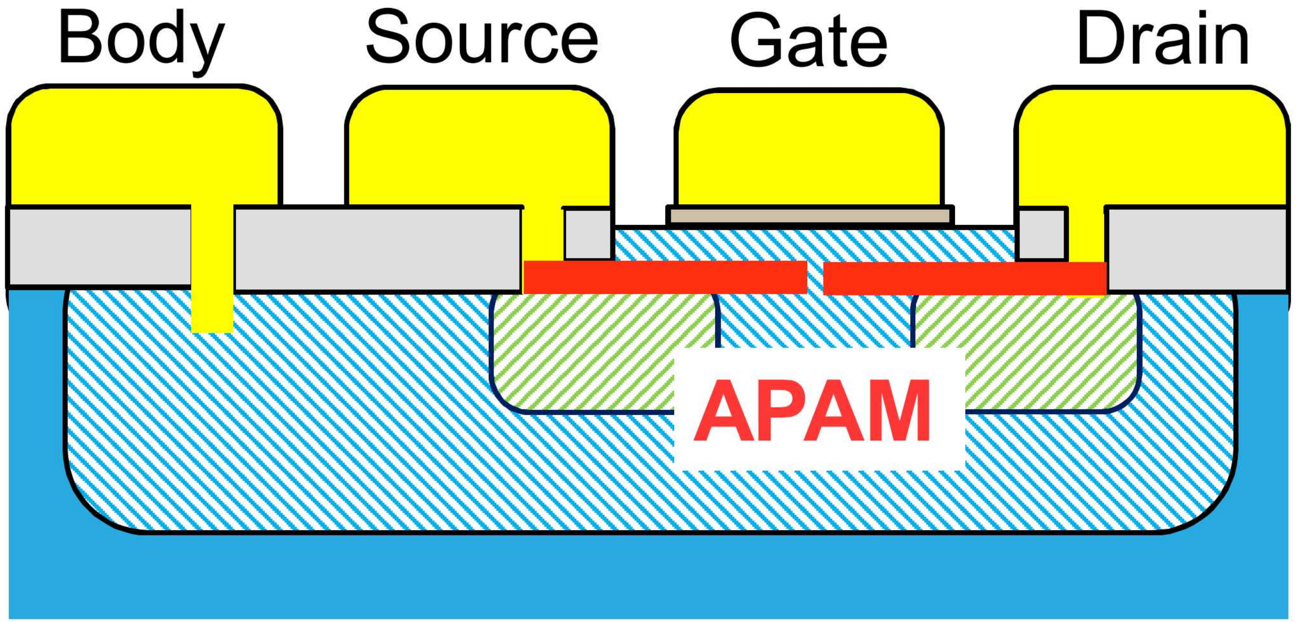
Take-away lessons

- Atomic precision does NOT mean atomically perfect
  - Dopant migration in APAM sample prep → need for new sample prep
  - Defects in silicon cap → bigger limitation than low-T oxides



- APAM needs new chemistries
  - Not just Si
  - Not just H
  - Not just PH_3