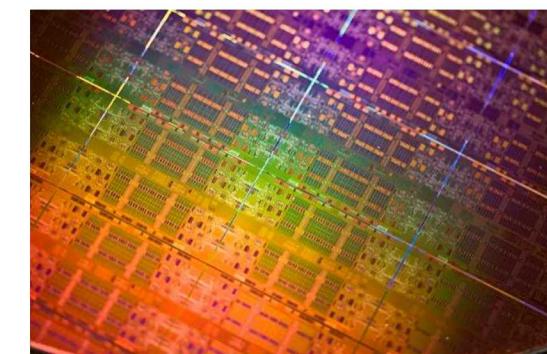
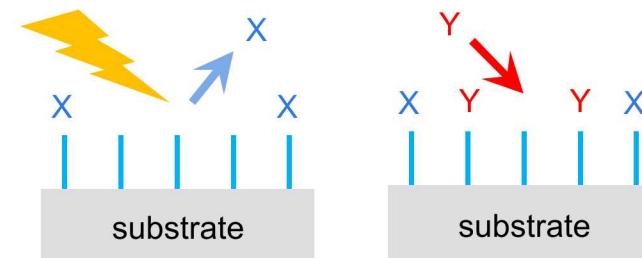
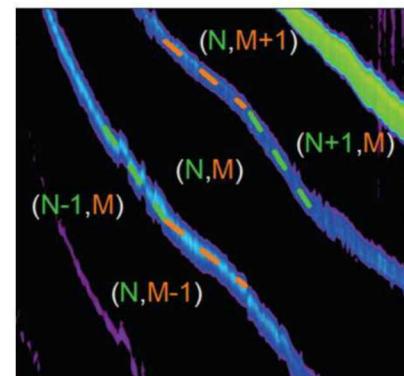
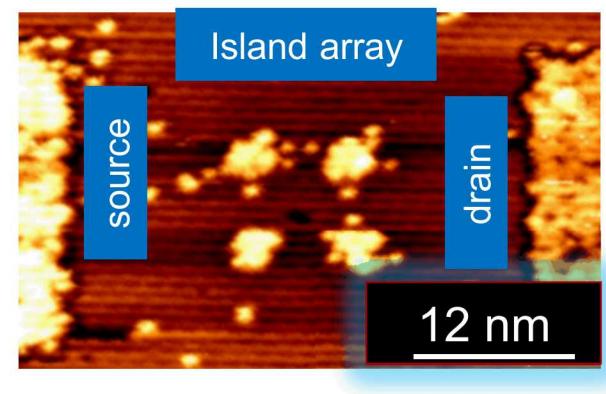


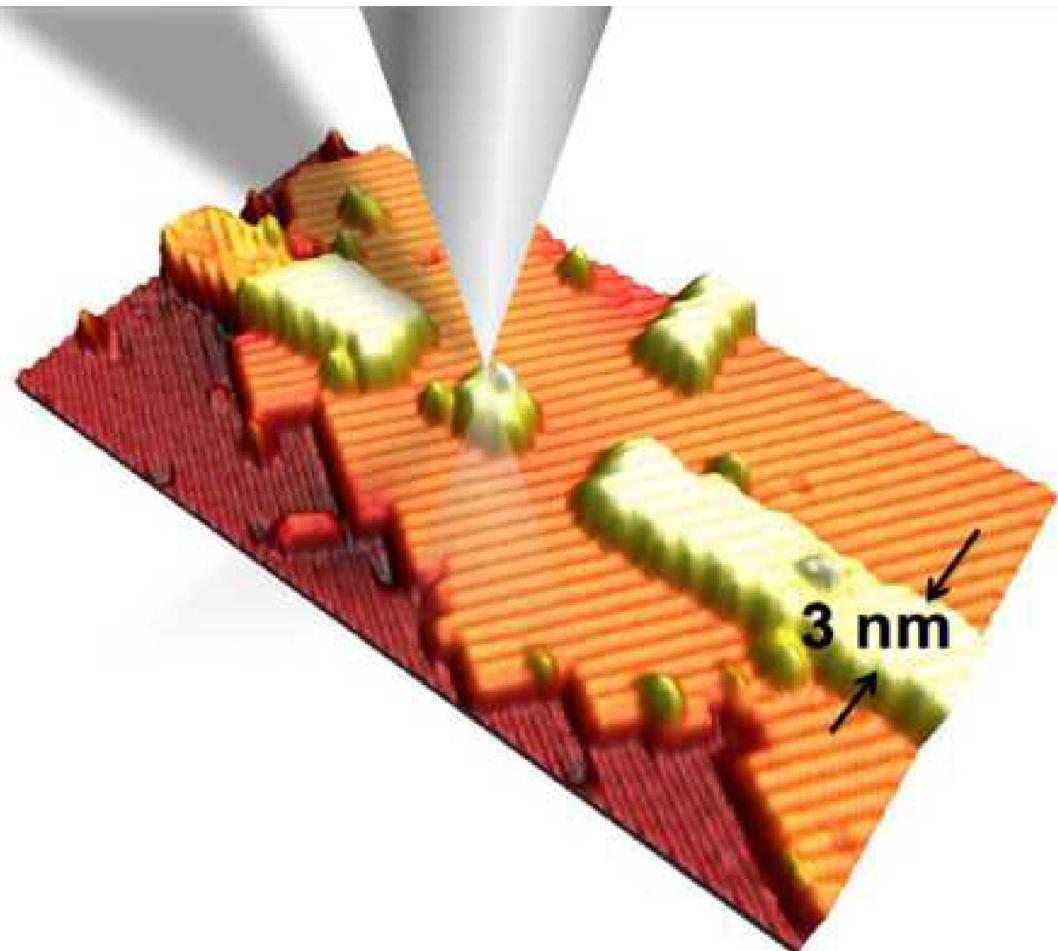
Quantum Electronics at the atomic scale: the next revolution?



Digital electronics at the atomic scale

Shashank Misra

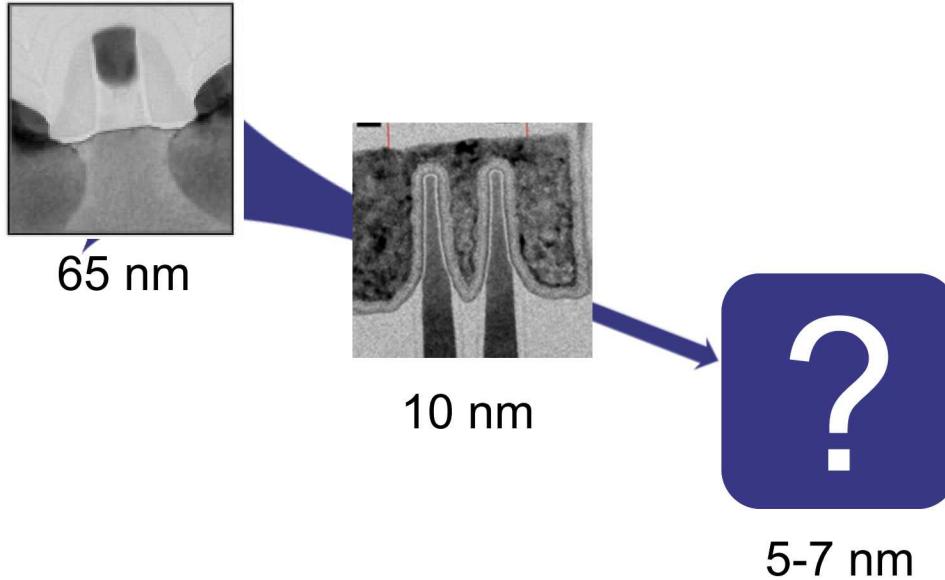
Atomic Precision Advanced Manufacturing



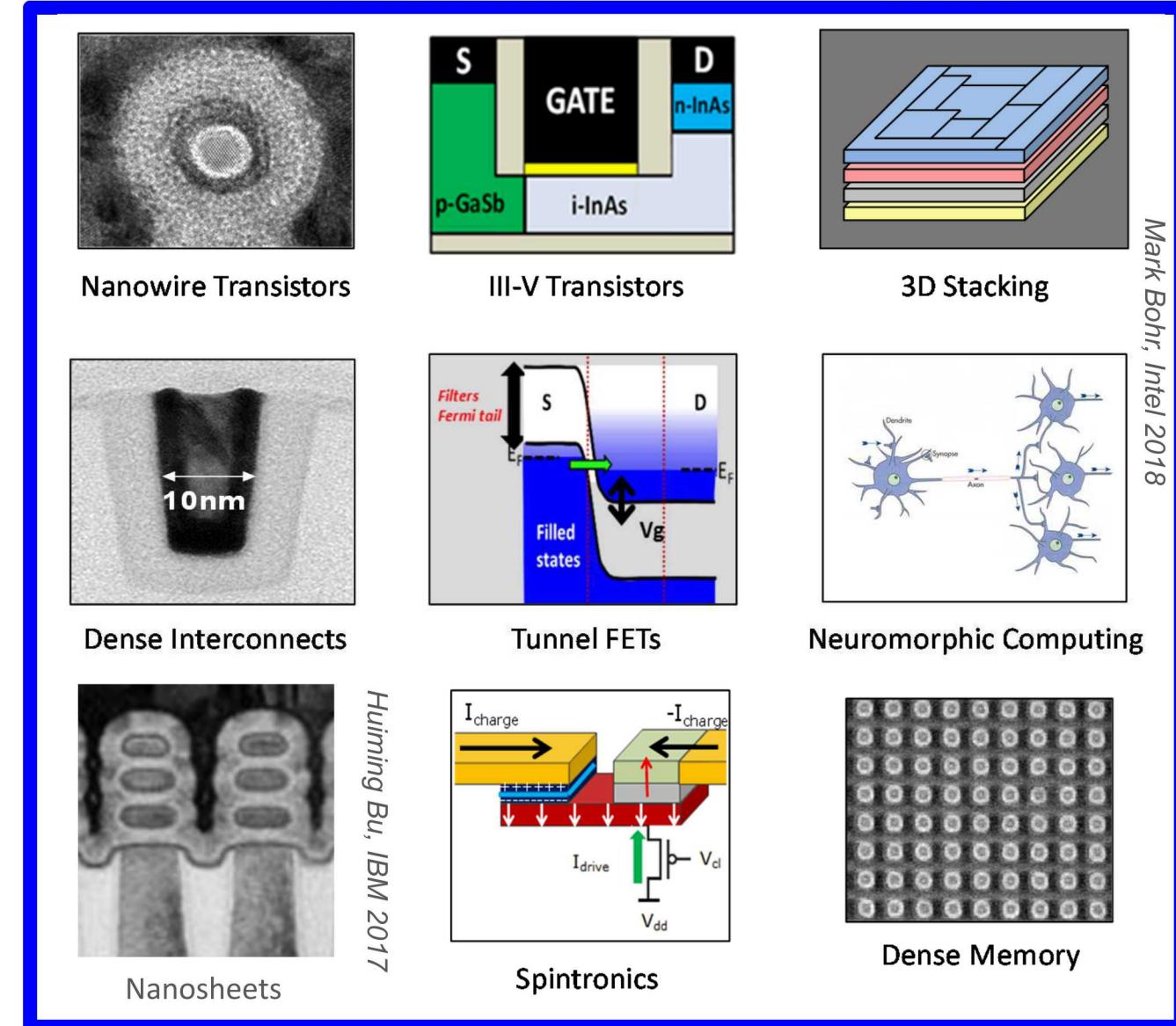
Assess the opportunities presented by having atomic-scale control over devices and processing for the digital microelectronics of the future

Where is microelectronics headed?

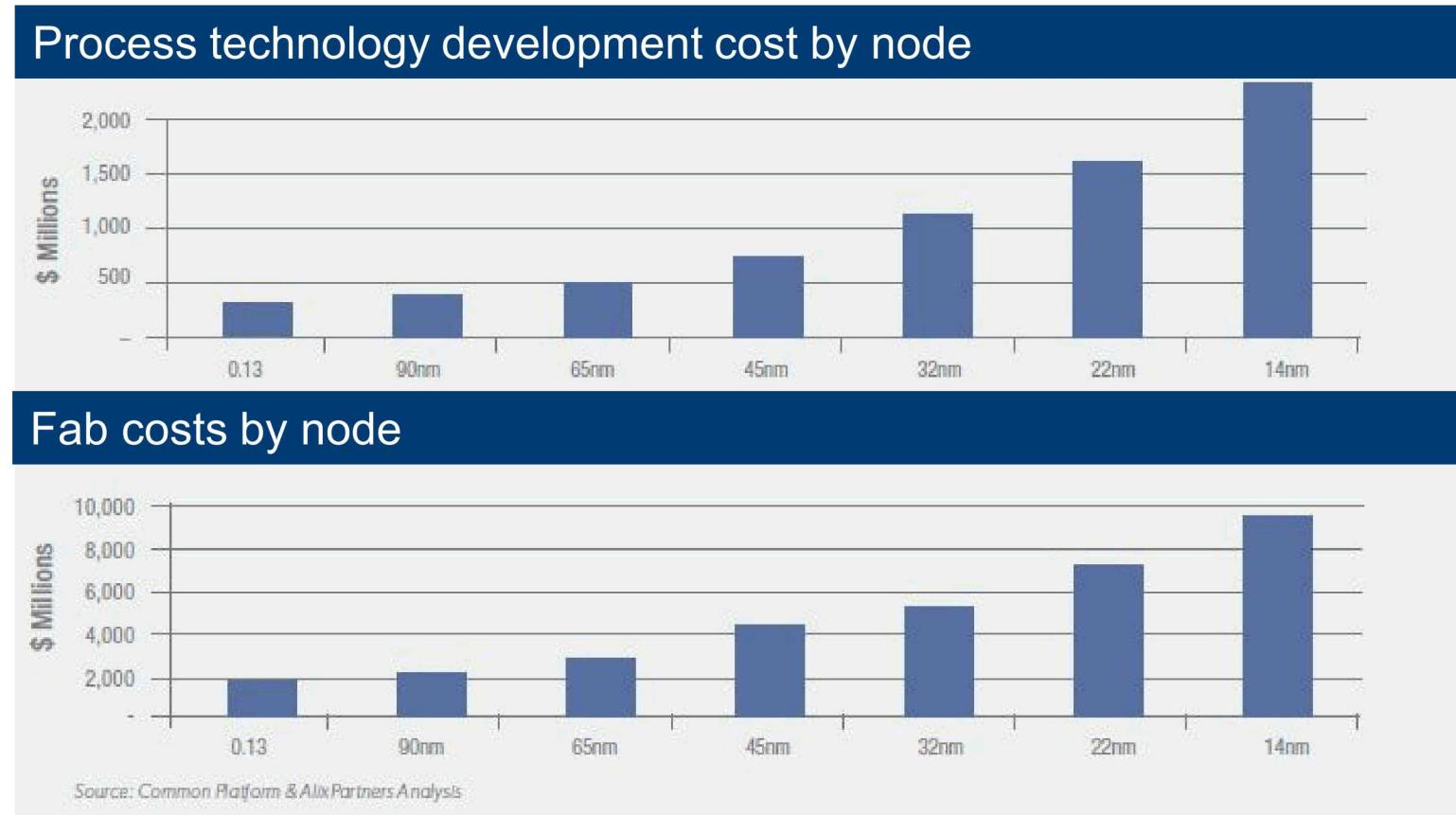
Historically, shrink transistor →
more functionality and declining cost



Unclear technology path.



Emerging risk in manufacturing-driven ecosystem

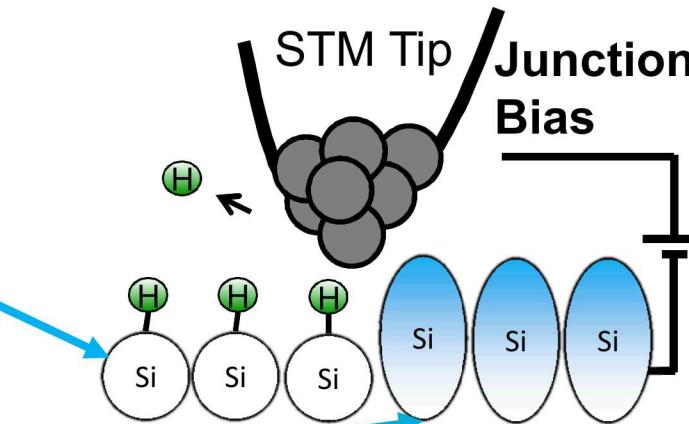
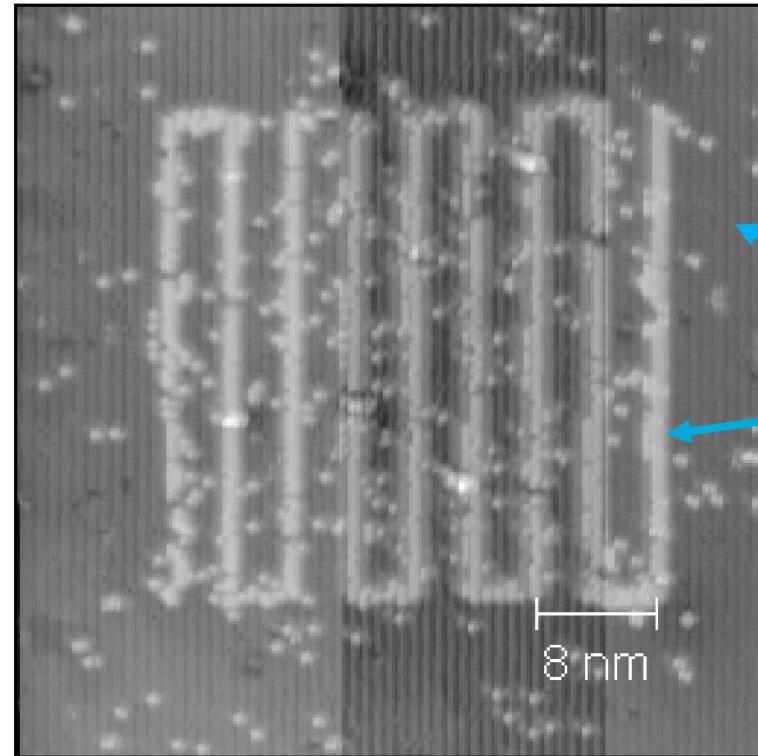


Ask what opportunities exist given atomic-scale control

How does Atomic Precision Advanced Manufacturing (APAM) work?

“Chemical contrast” at Si surface

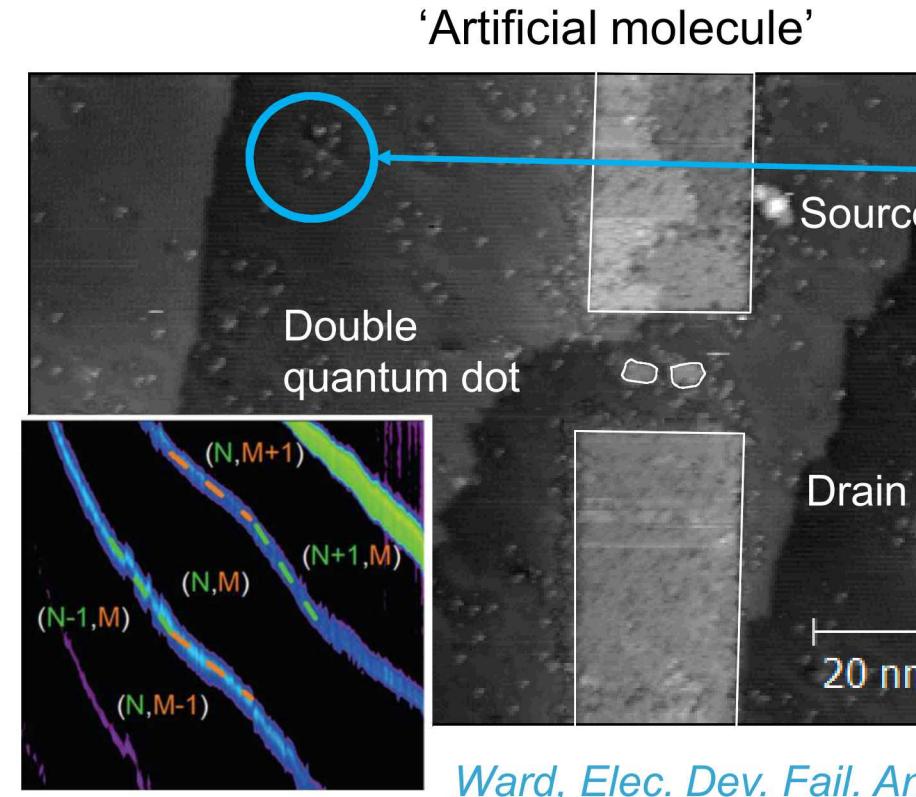
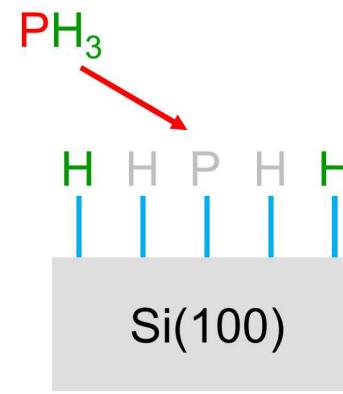
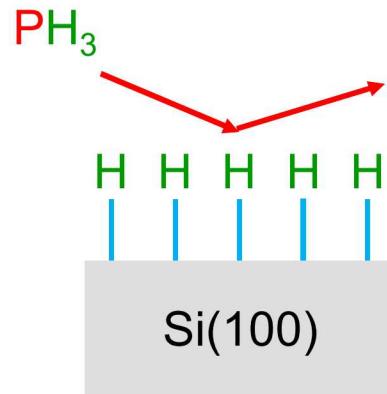
- Unterminated Si: 1 reactive bond/ atom
- H-terminated Si: unreactive



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

Area-selective chemistry with phosphine

Phosphorus 'donates' an electron to silicon.

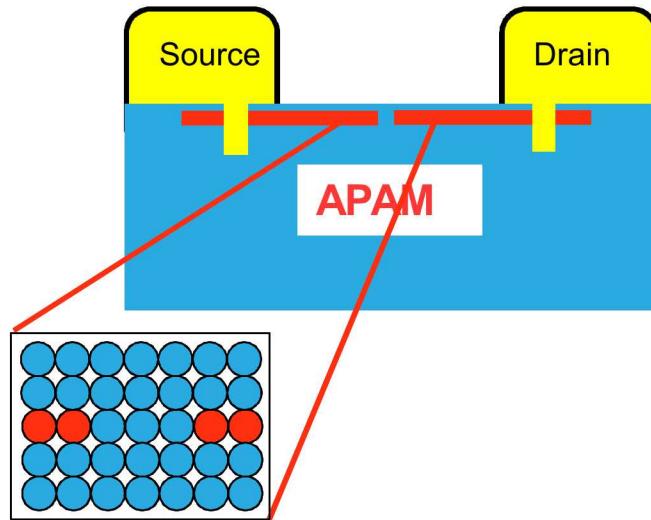


[Ward, Elec. Dev. Fail. Anal. \(2020\)](#)

Opportunities outside of quantum demonstrations
Opportunities outside of atomic-scale widgets

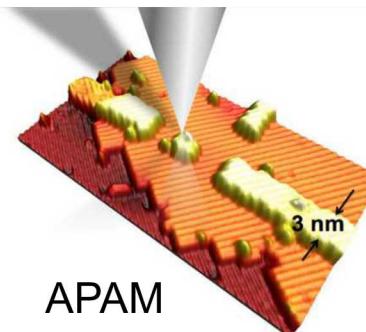
How to get to digital electronics at the atomic scale?

1. APAM devices



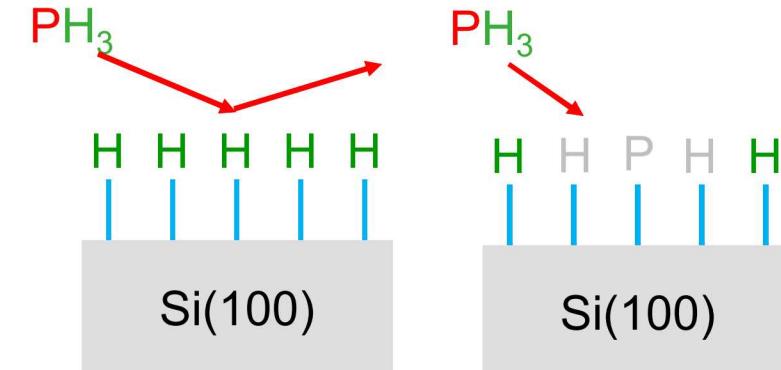
- Simple planar devices
- Only work at cryogenic temp.

2. CMOS integration



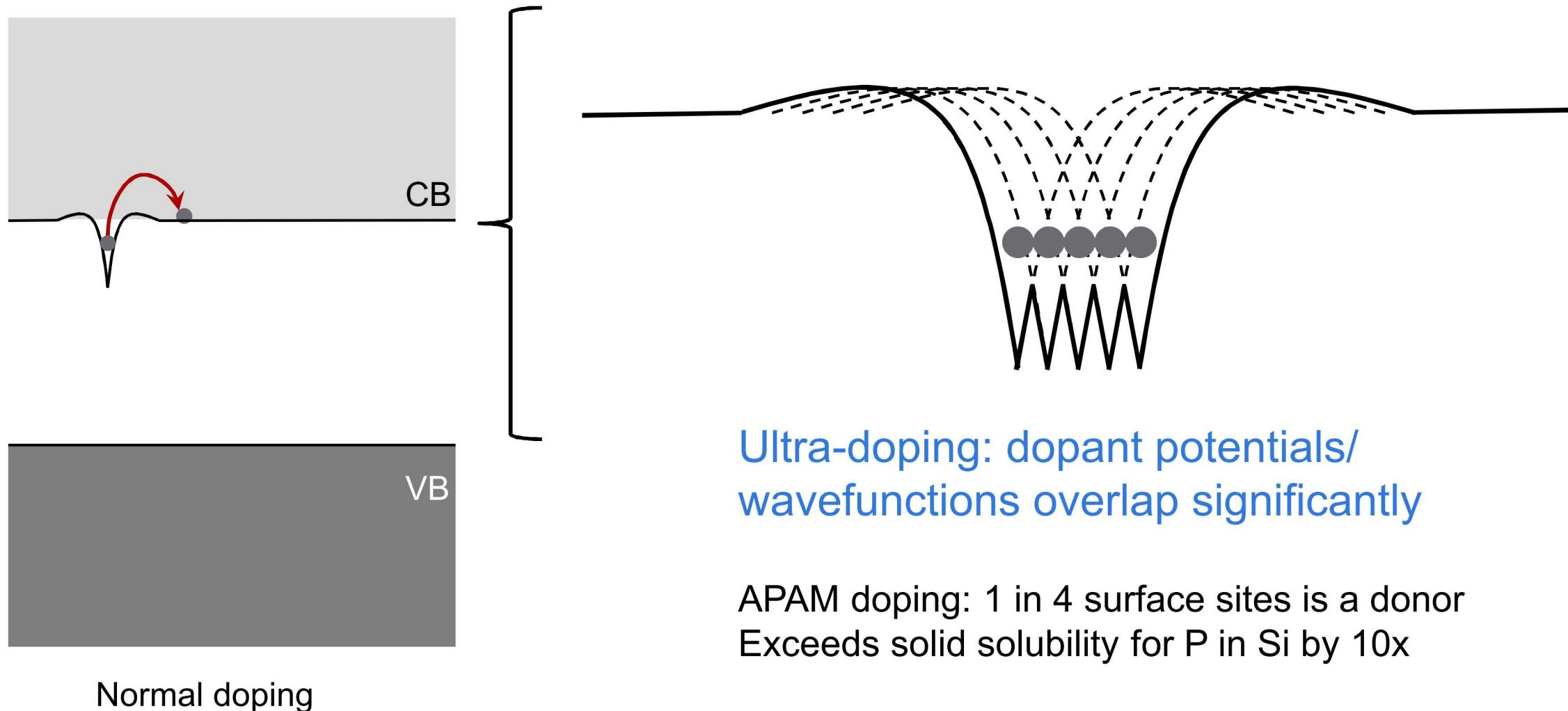
- Incompatible with CMOS workflows / parts

3. APAM toolkit

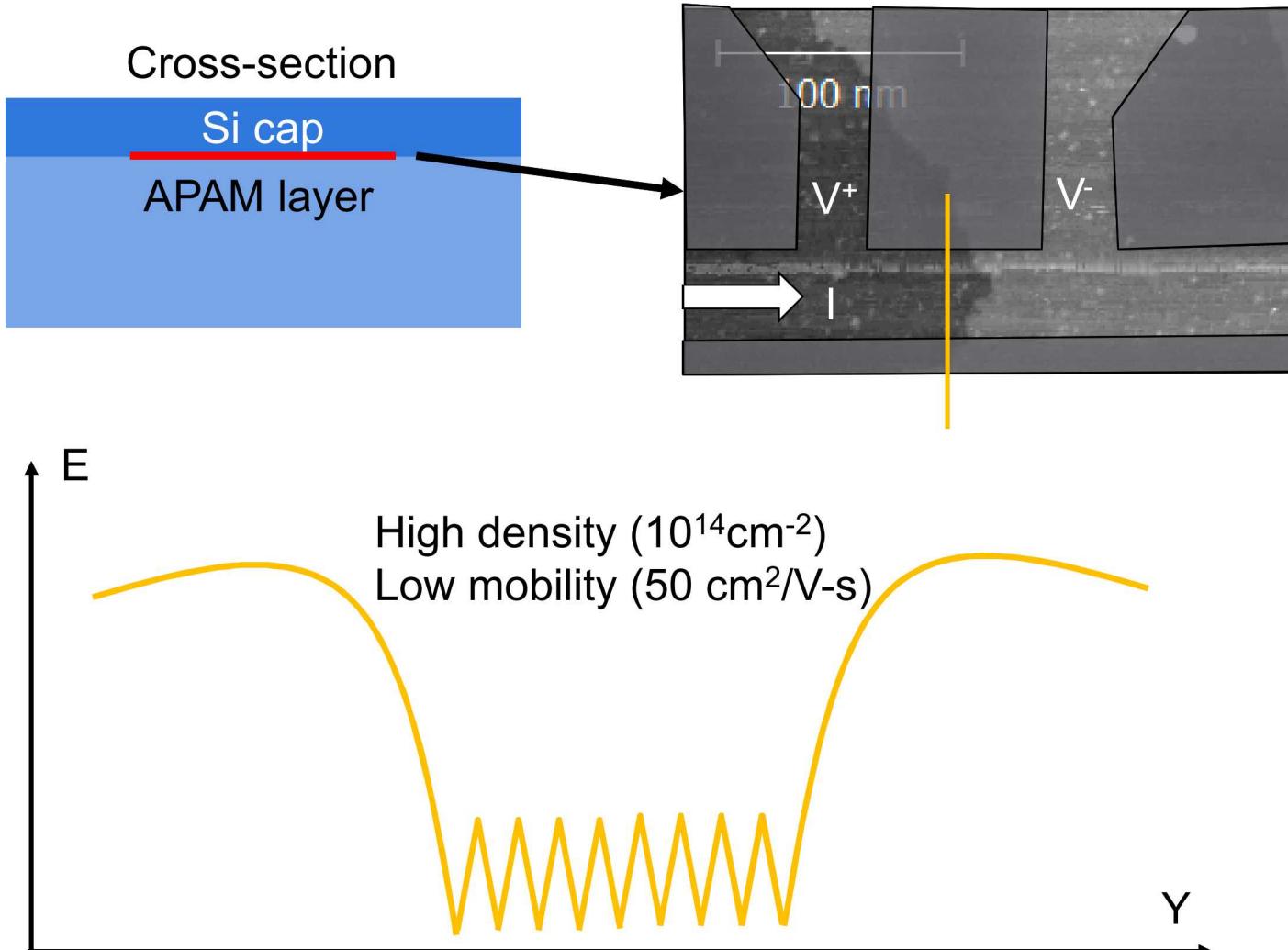


- One working chemistry

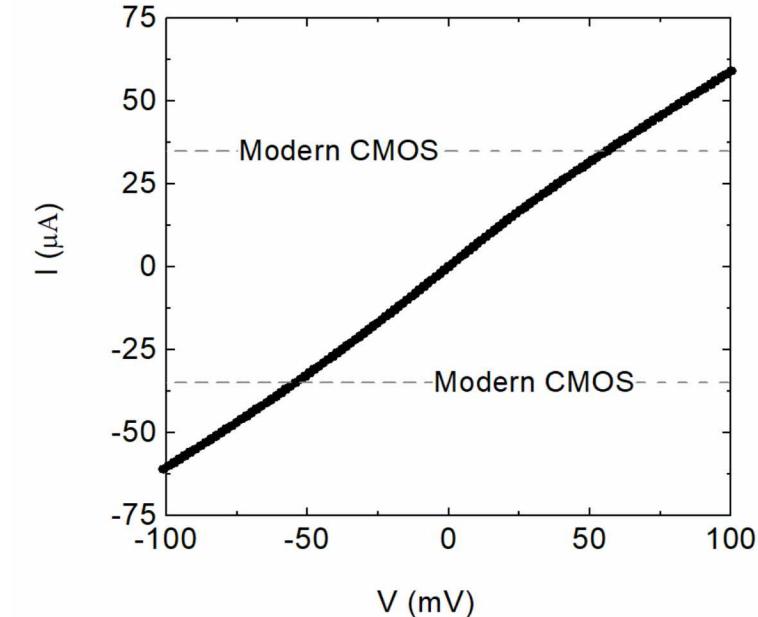
What does APAM do that's special? “Ultra-doping”



Consequences: confinement

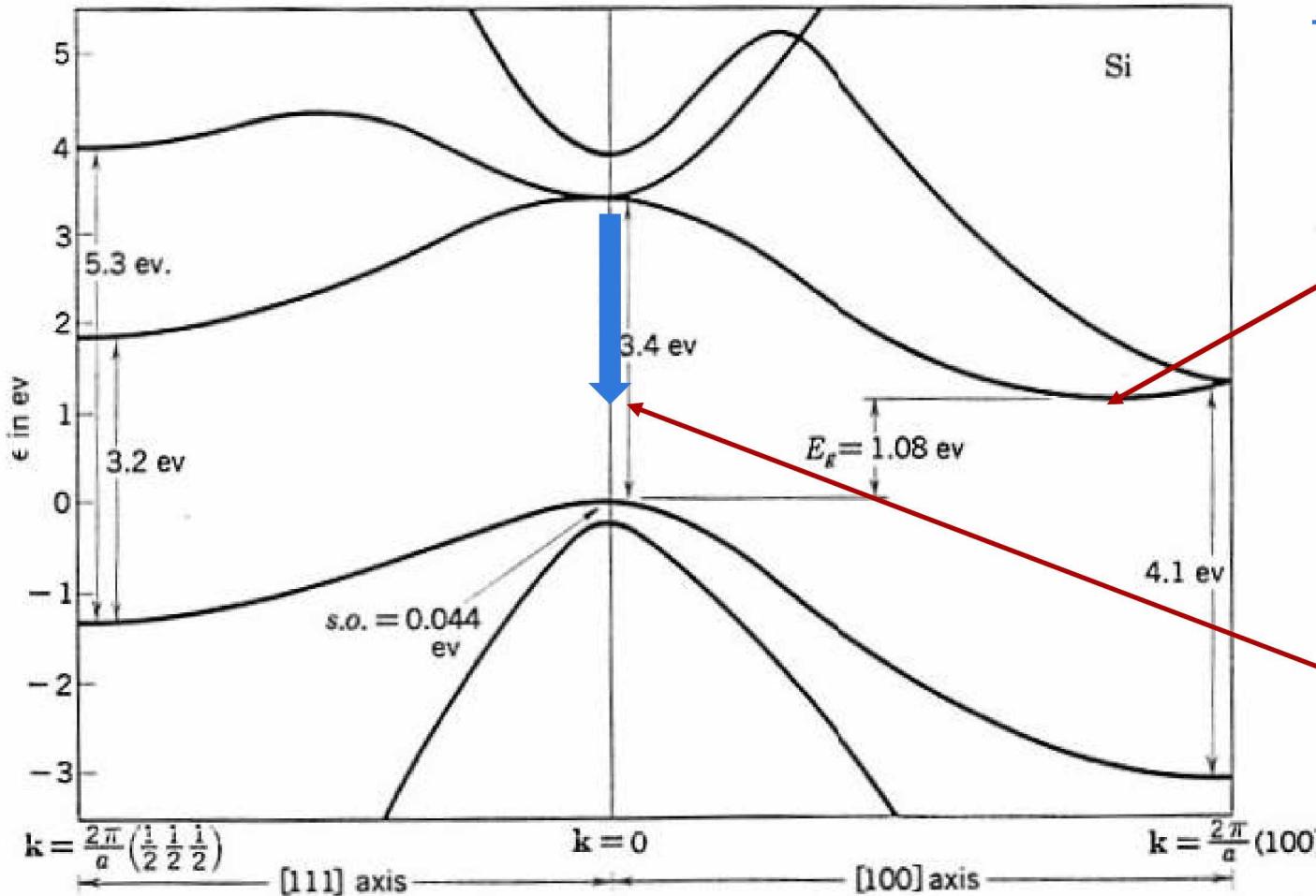


[Ward, Elec. Dev. Fail. Anal. \(2020\)](#)

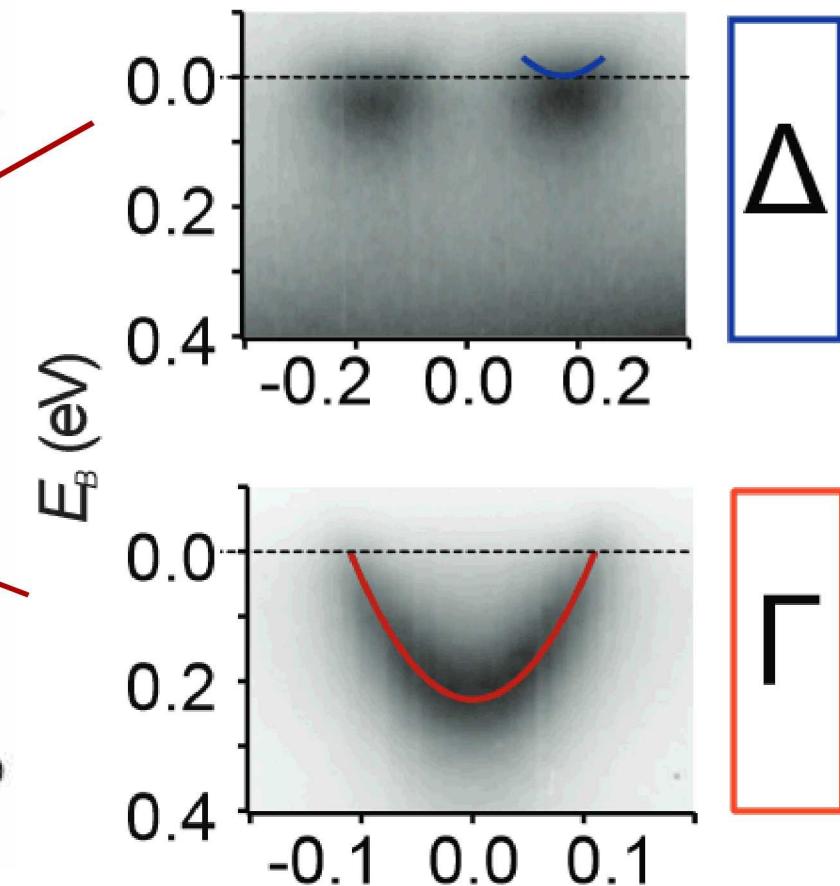


Dopants give you confinement
Extremely high current density.

Consequences: electronic structure

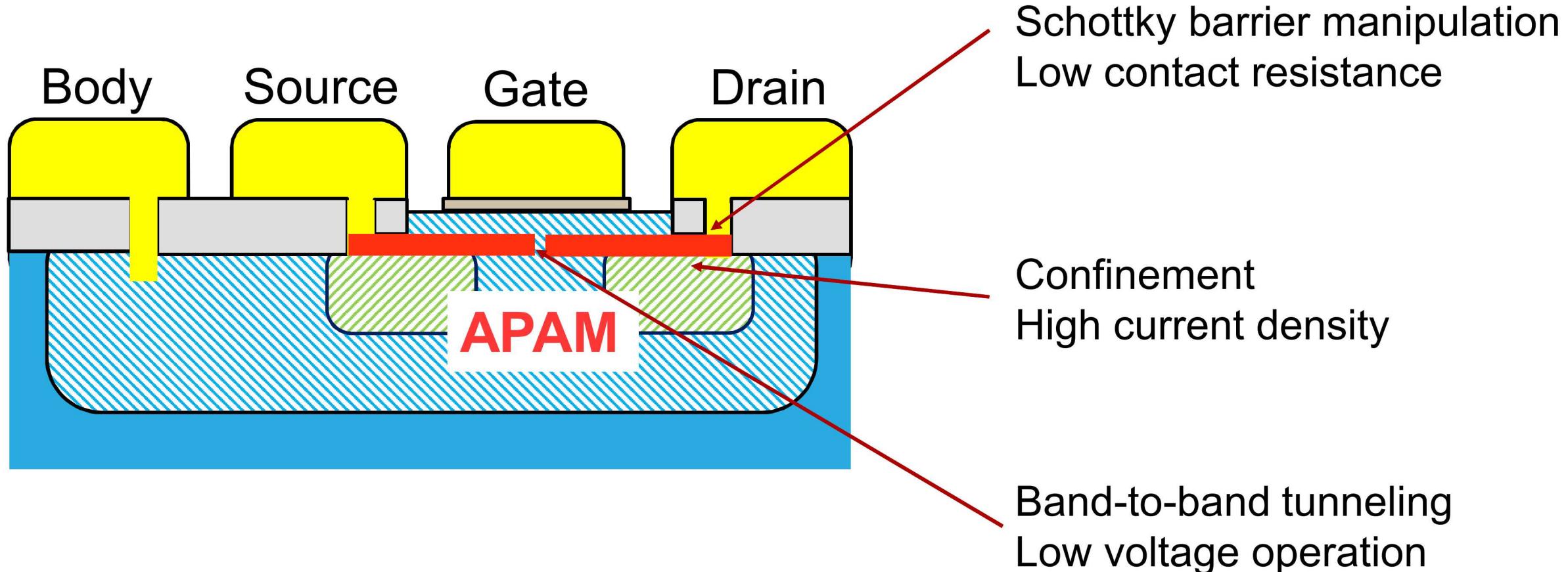


This isn't really silicon like you know it.



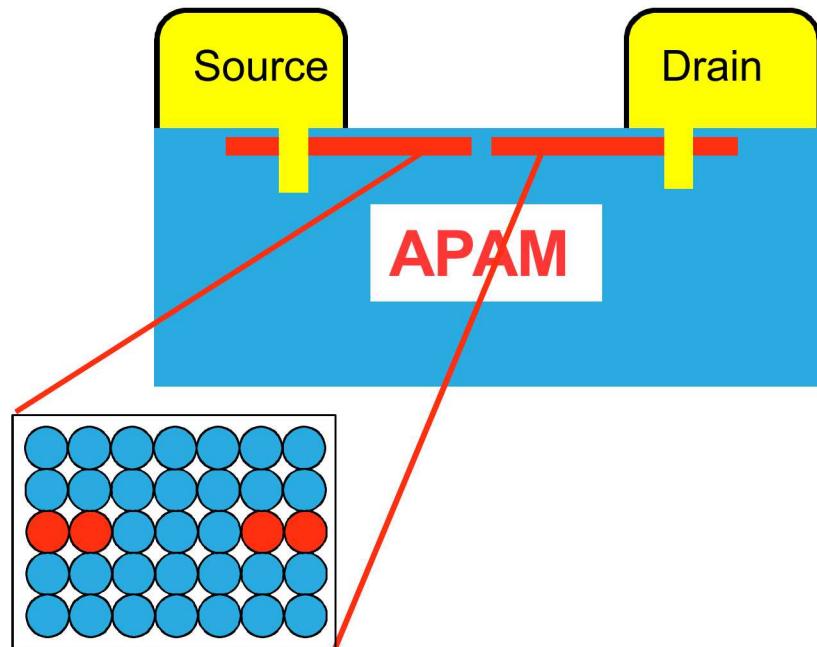
[Holt, arXiv:1911.08274](https://arxiv.org/abs/1911.08274)

APAM-inspired transistor

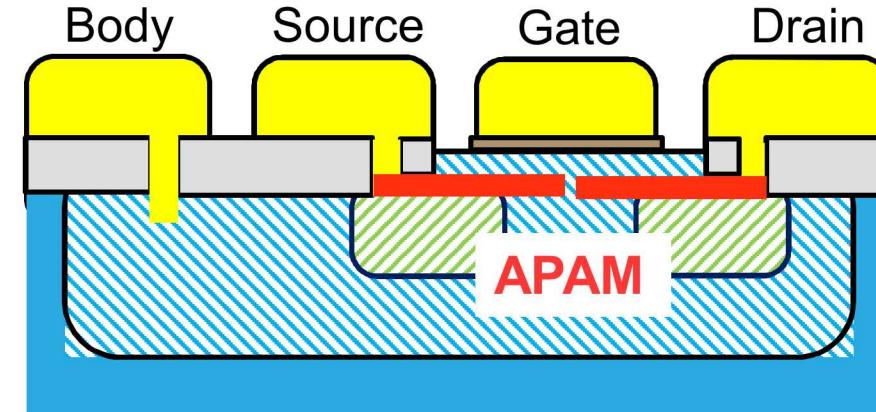


Can you make a 'real' transistor with APAM?

Now (3 US labs, 6 labs worldwide)



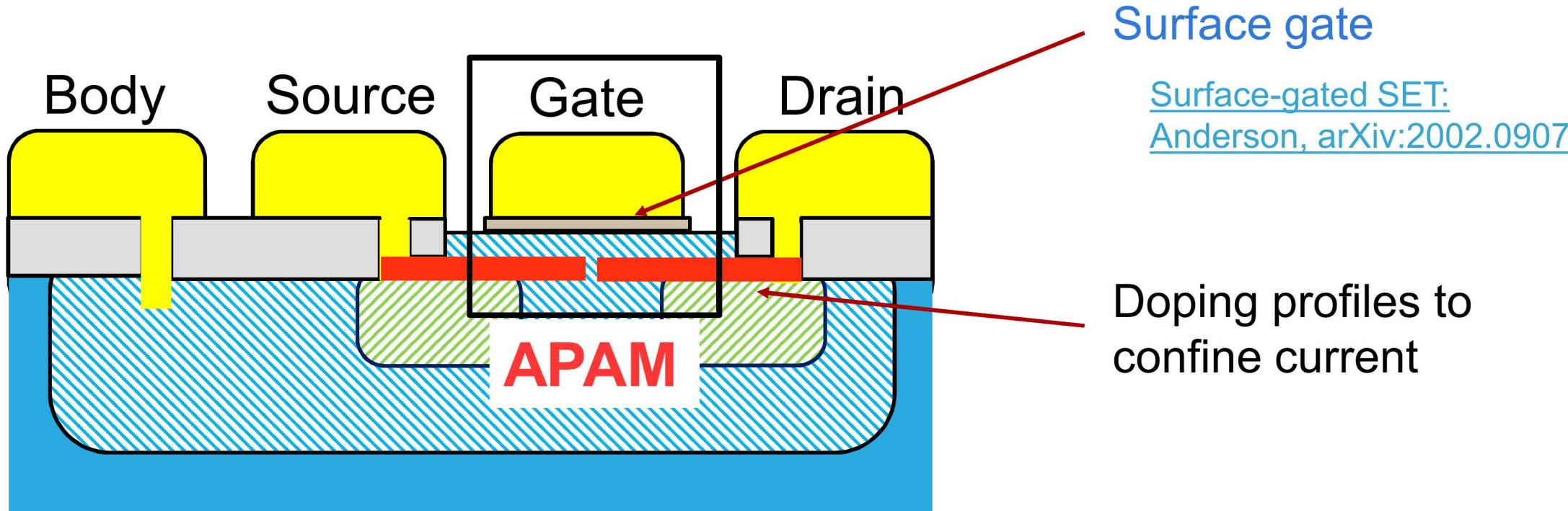
Desired future state



- Only works at cryogenic temperatures
- Devices consist only of phosphorus!

- Works above room temperature
- Device is complex

“Real” APAM transistor

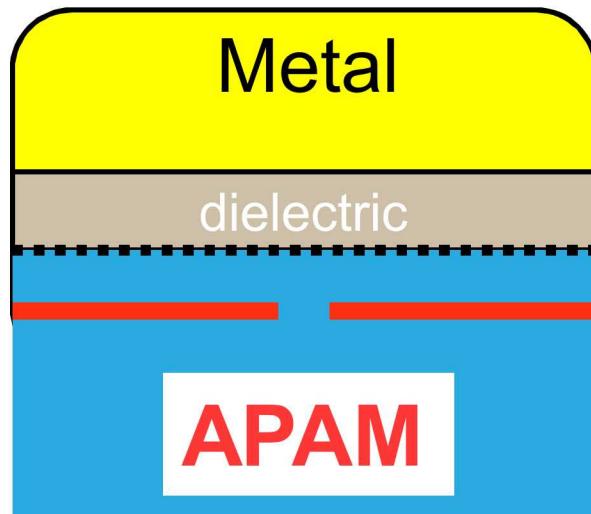


Surface gate challenge: thermal budget

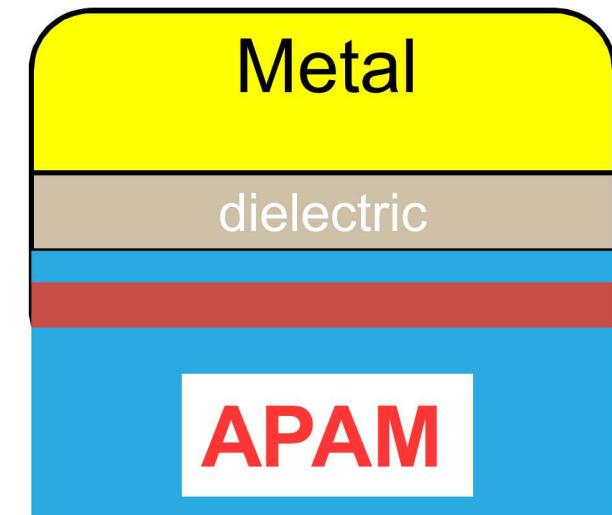
Dopants readily diffuse ~ 350 – 550 °C
Low defect silicon oxide needs ~ 800 °C

Modern high-k dielectrics require temperatures that are accessible

Low temperature



High temperature

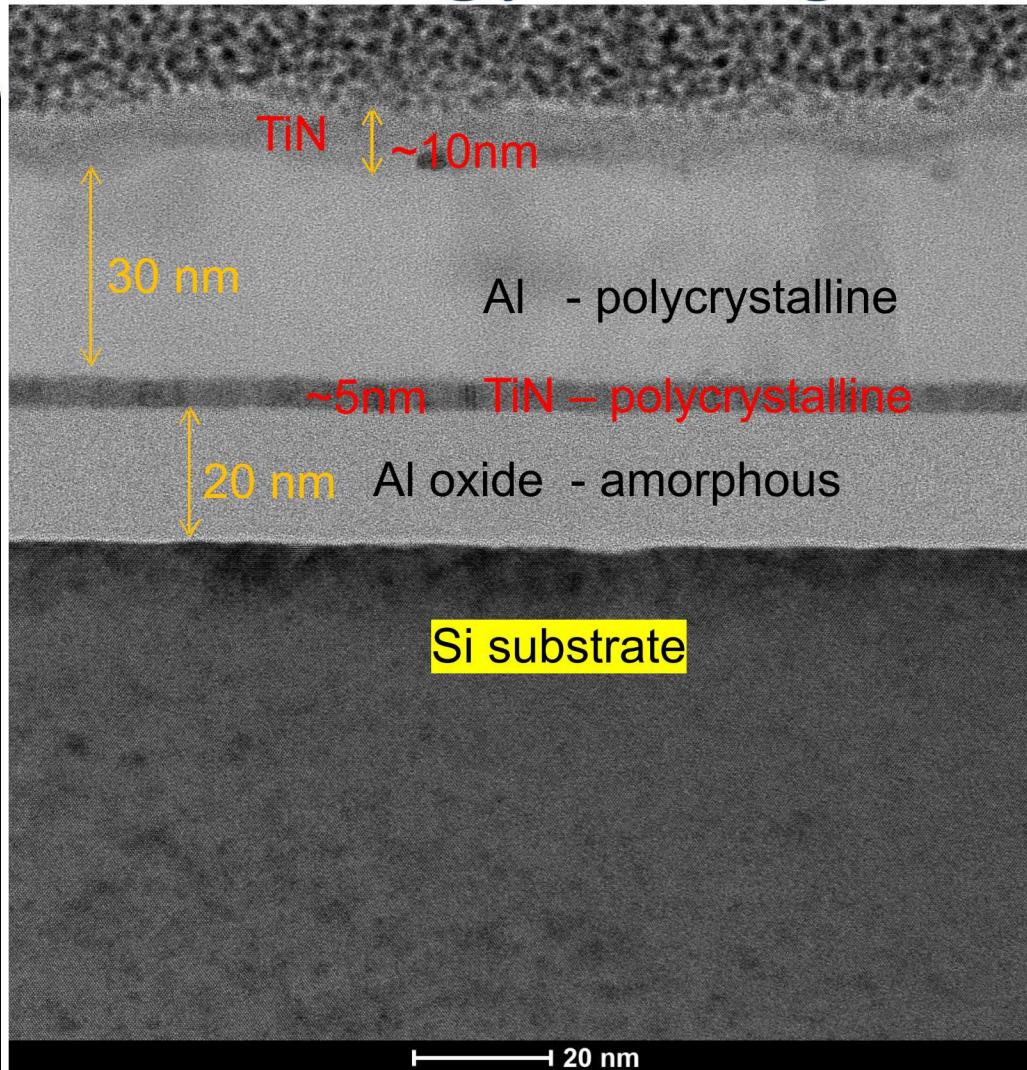
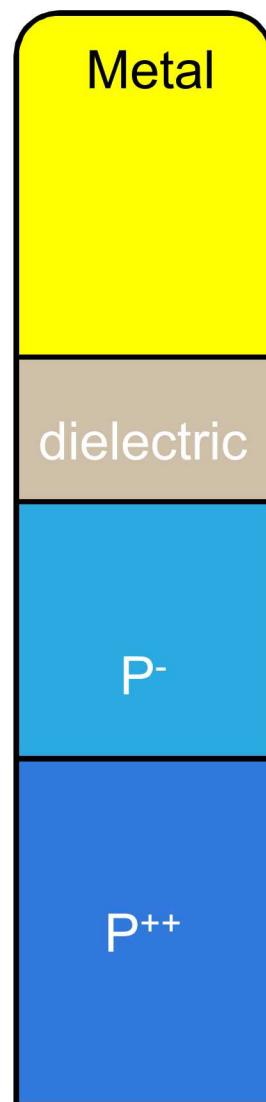


Is there a sweet spot?

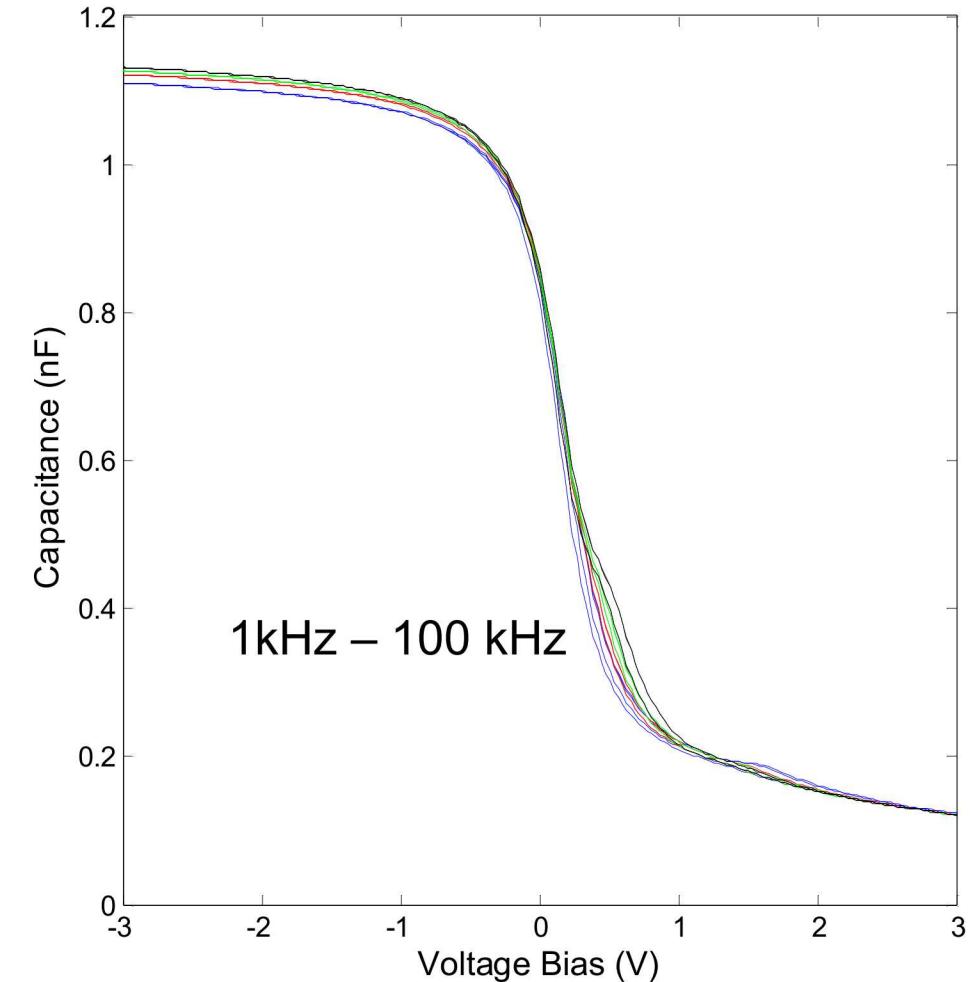
Poor quality interface shields gate
Dopants have remained in place

High quality interfaces
Dopants have diffused

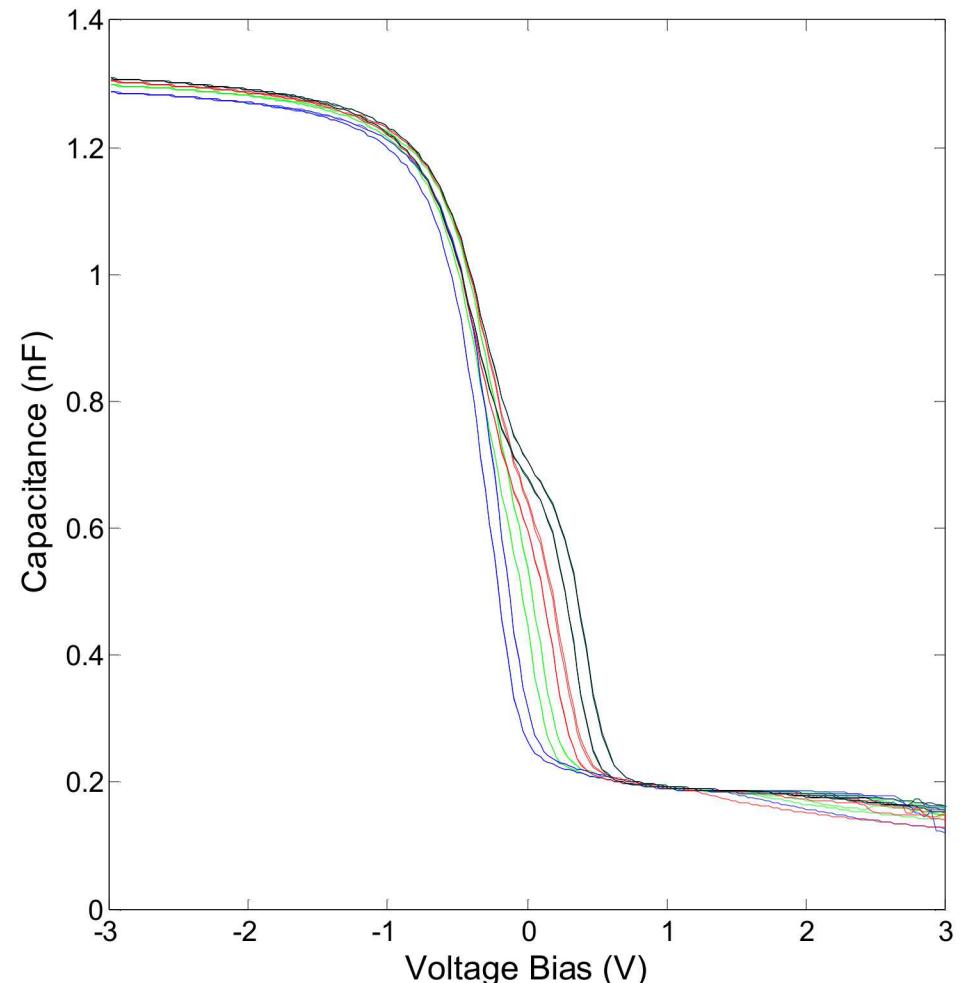
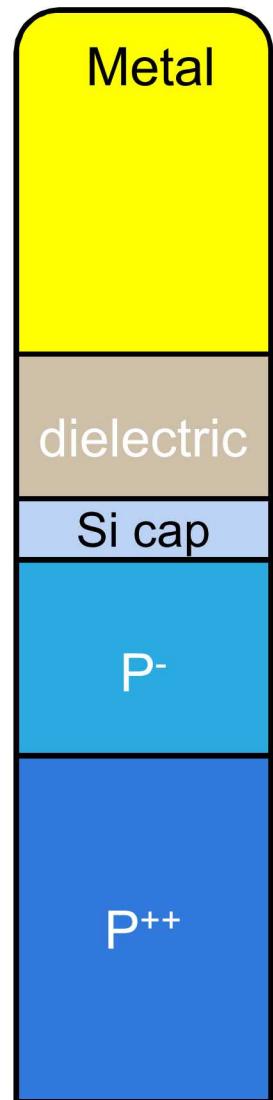
Follow strategy for high-k/metal gates



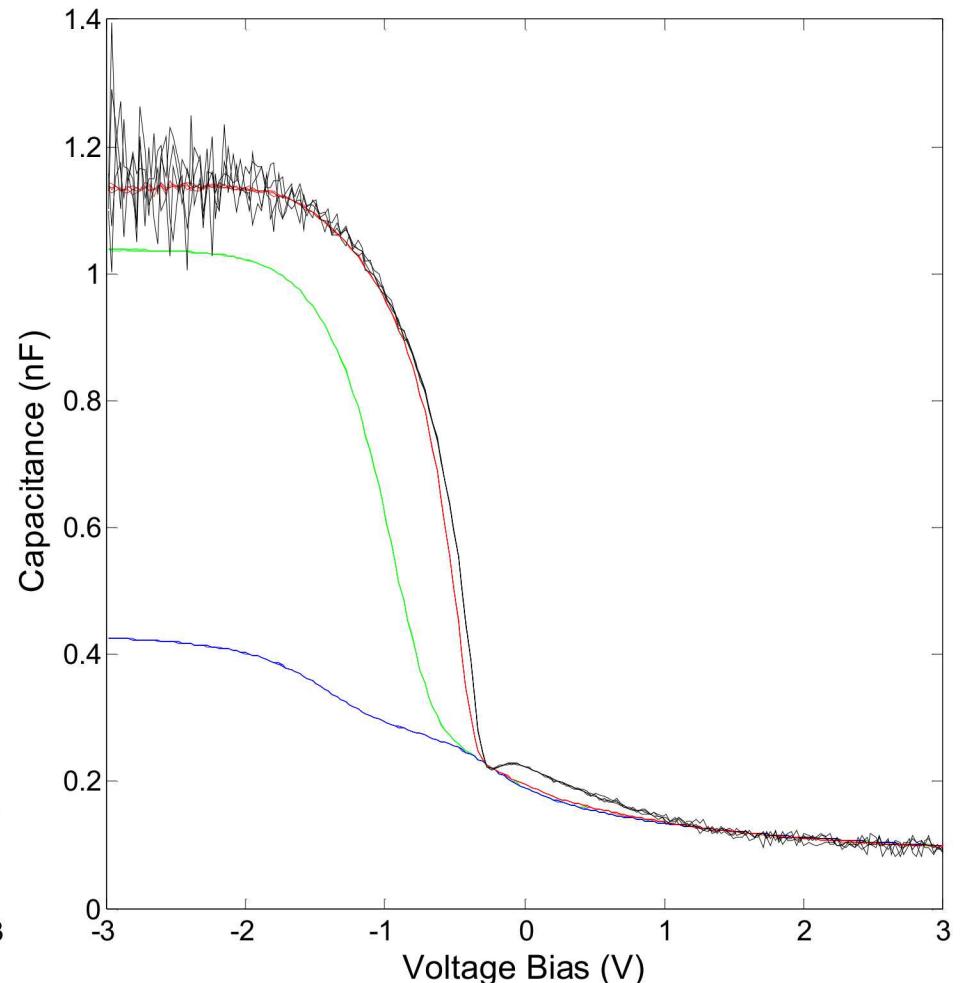
Thermally compatible with APAM (250 °C). Low density of interface defects: $4 \times 10^{10} \text{ cm}^{-2}$



First-ever CV curve on an APAM layer



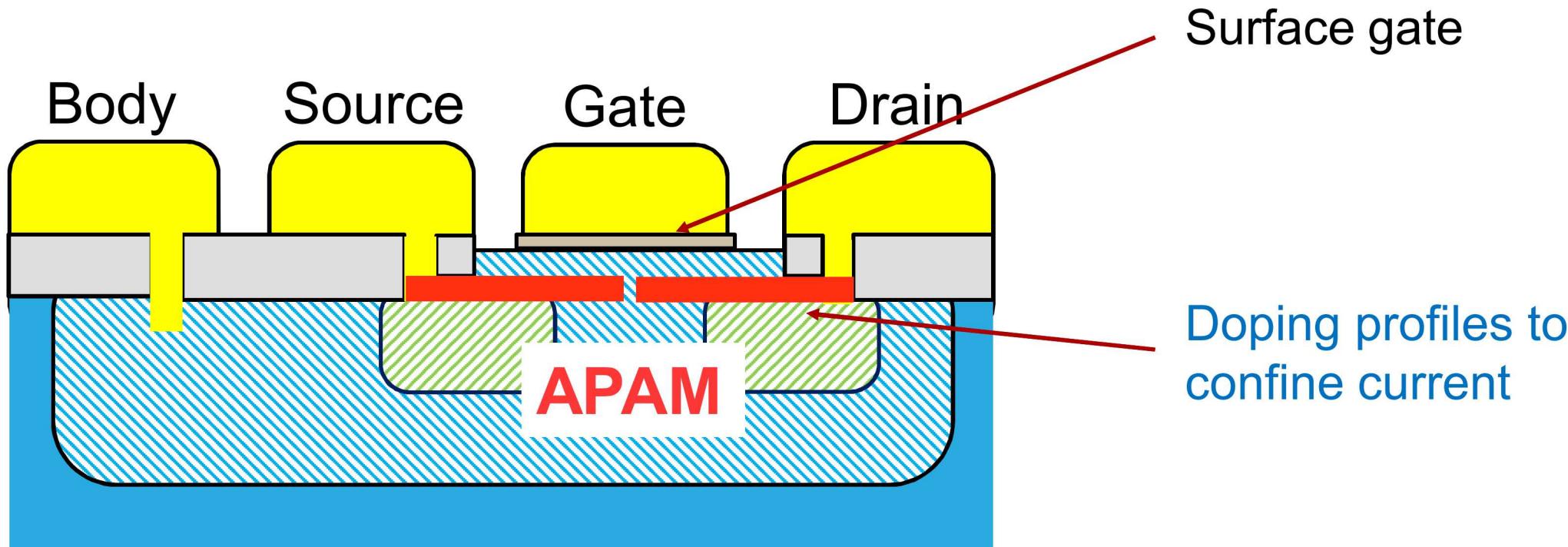
Surface charge: $1 \times 10^{11} \text{ cm}^{-2}$



Soon: finite frequency TCAD model



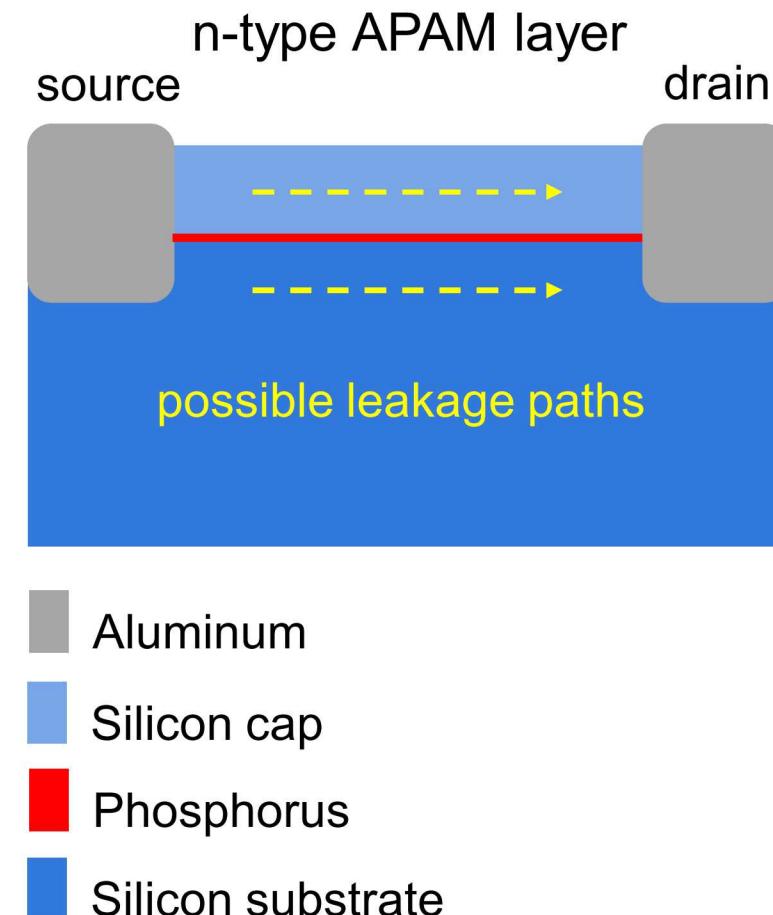
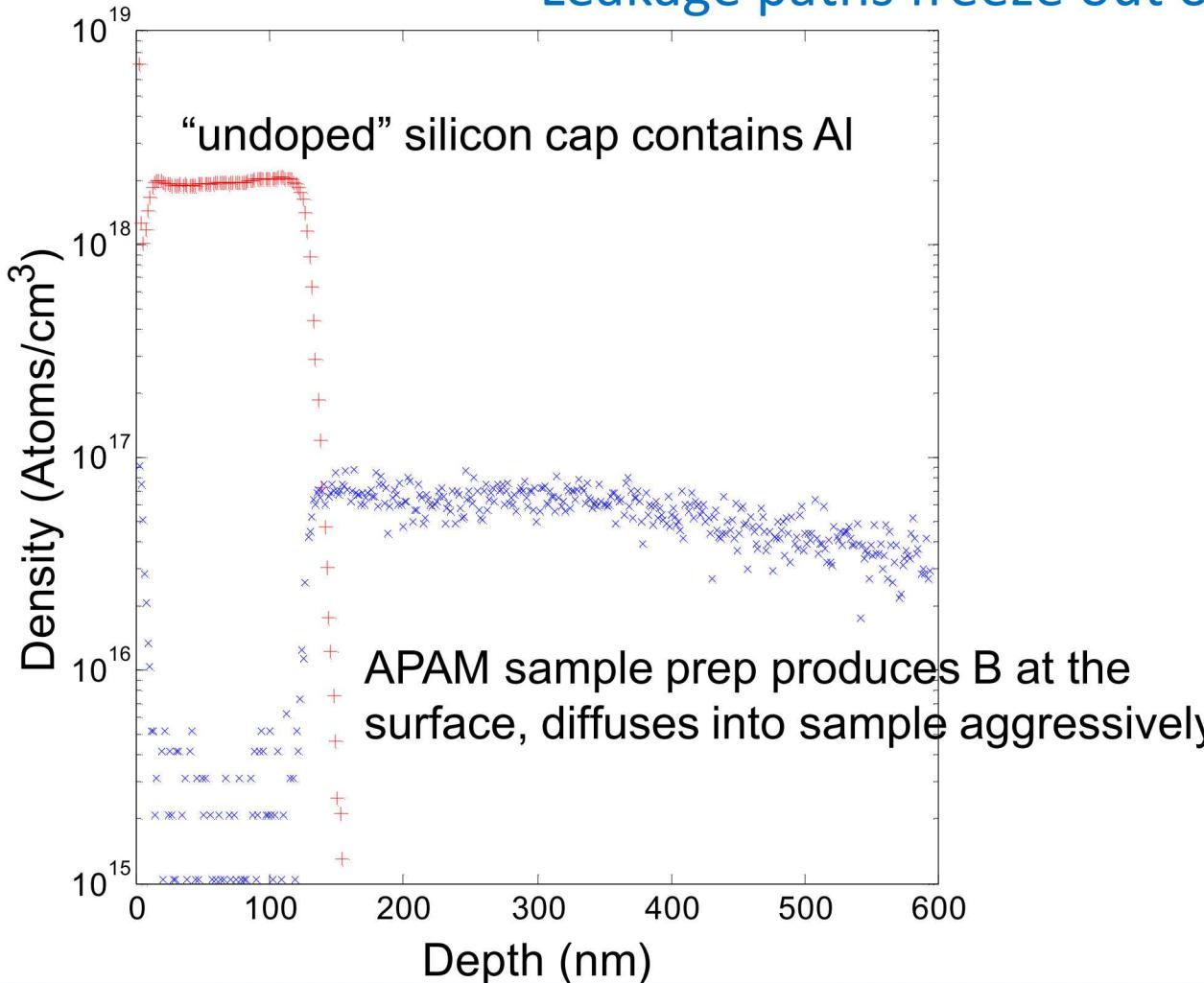
“Real” APAM transistor



Room Temperature Device Operation

Unintentional doping of cap and substrate

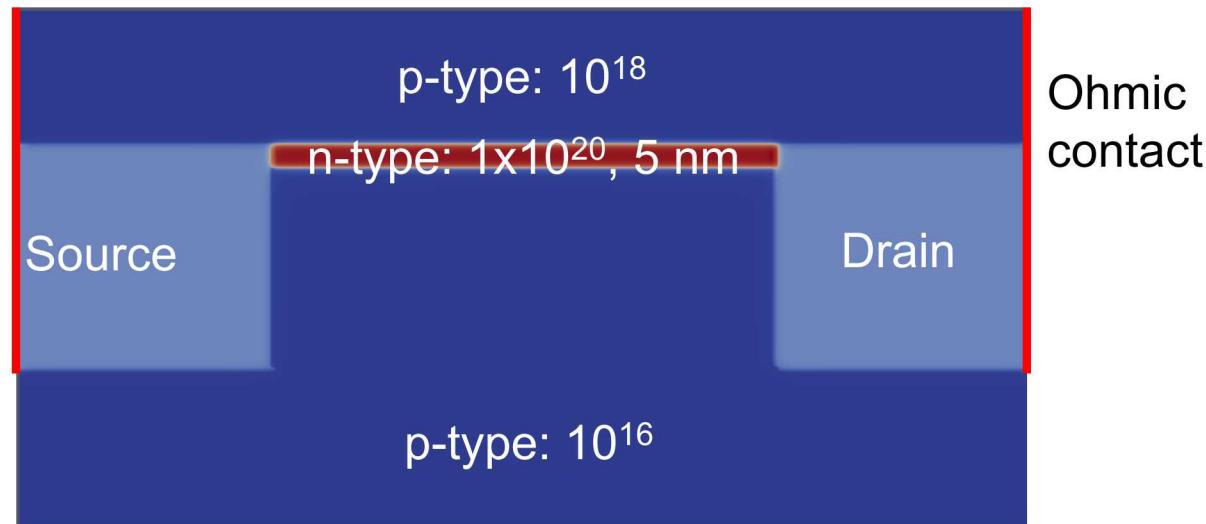
Leakage paths freeze out only at low temperatures



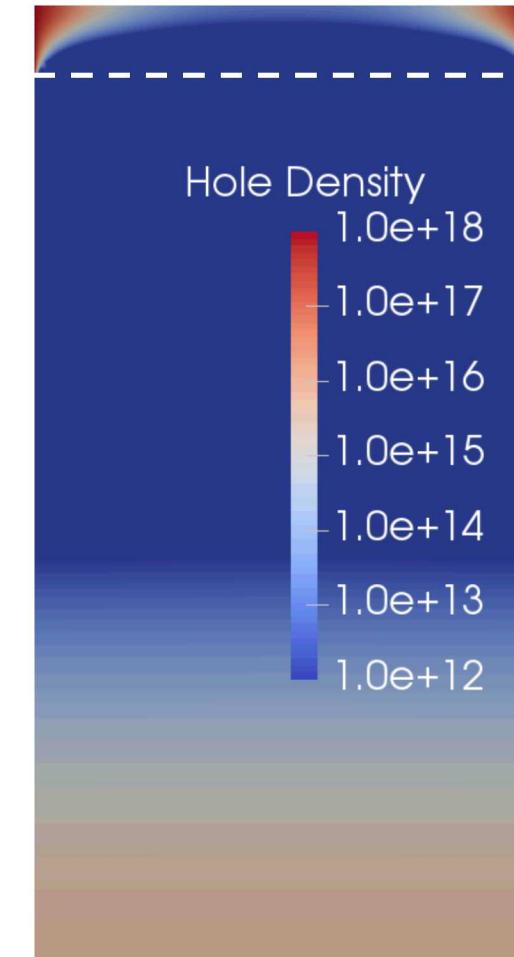
TCAD Simulations

APAM layer depletes the substrate and cap

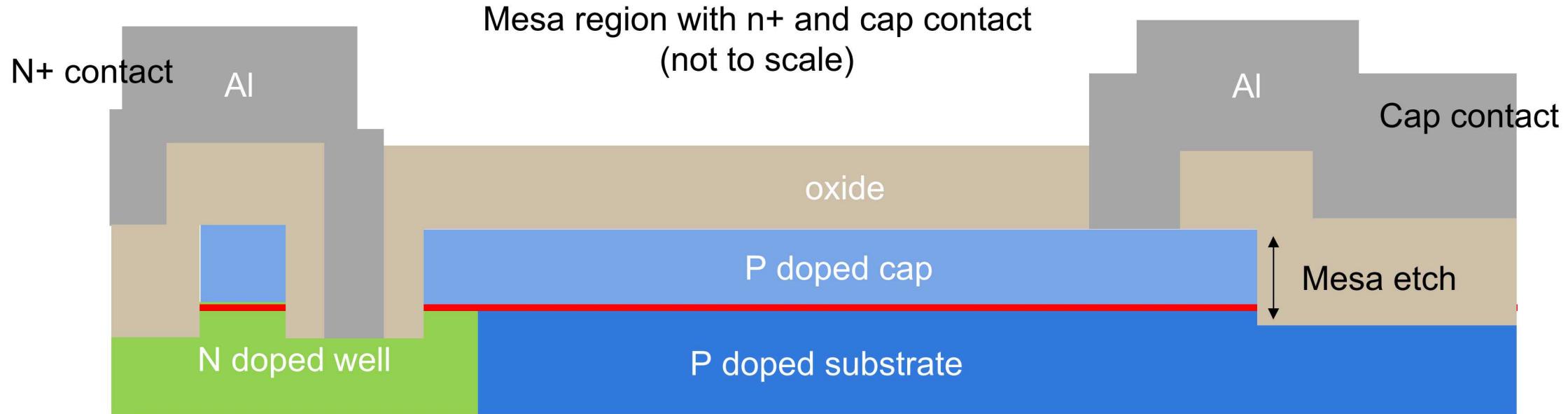
Simulation Structure



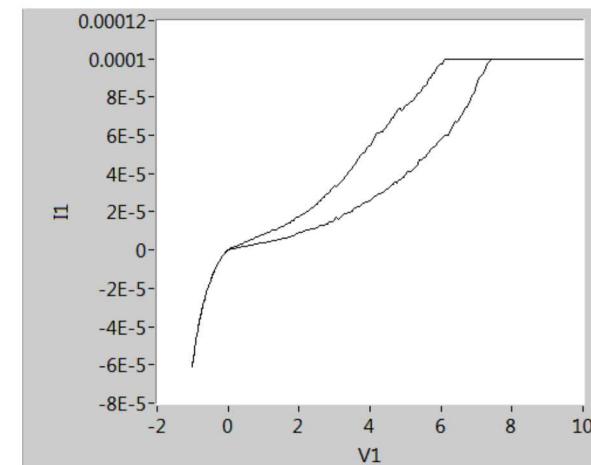
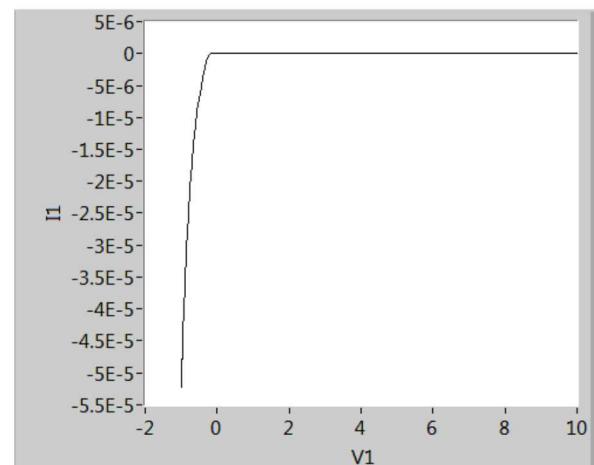
Hole Density from TCAD



Contact isolation

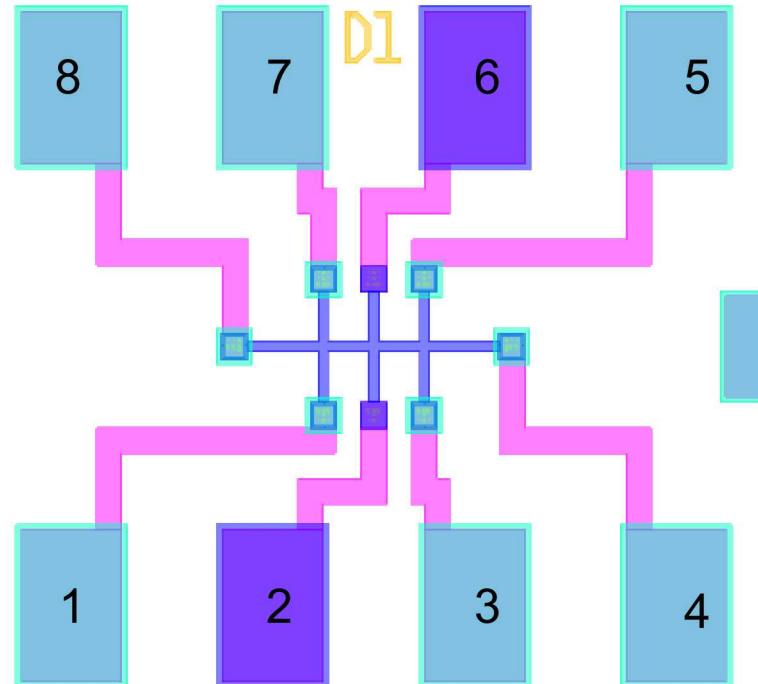


After wire bonding
25 g force



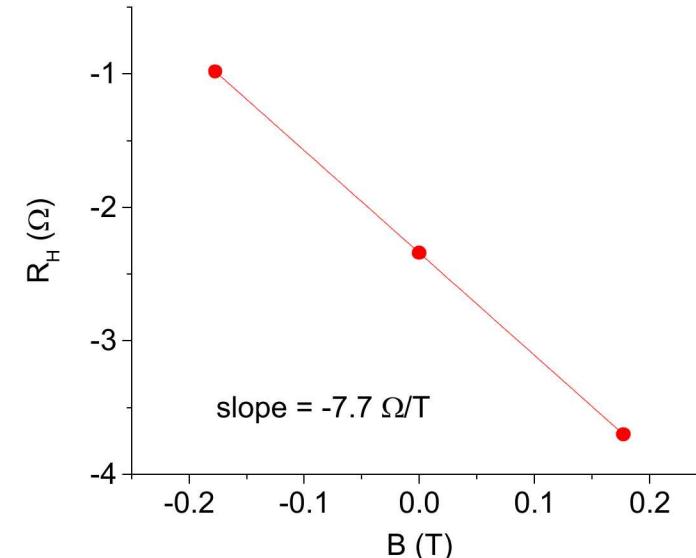
After wire bonding
35 g force

1st measurement of APAM wire at room temp.



R_{xx} : 4.80 mV/450 nA

(20-40 nA leakage at 1V)



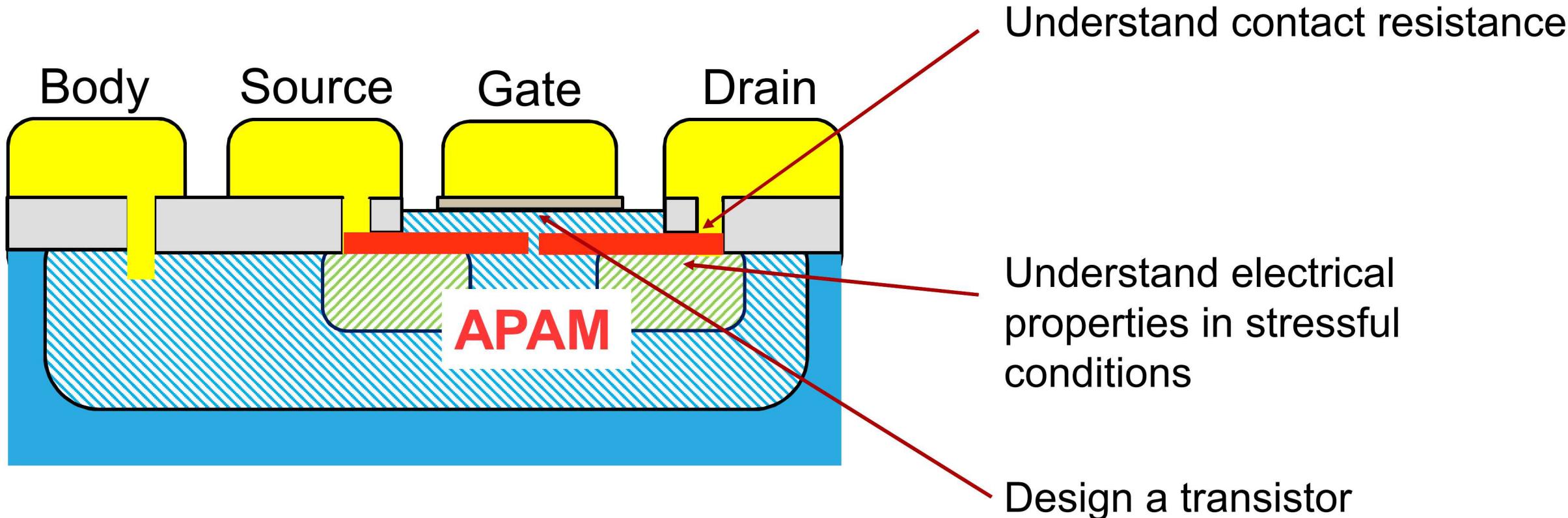
Temperature	Resistivity	Carrier density	Mobility
4 K	600 Ω/sq	$1.7 \times 10^{14} \text{ cm}^{-2}$	55
293 K	1070 Ω/sq	$0.8 \times 10^{14} \text{ cm}^{-2}$	65

Unclear why density goes down,
mobility stays same.

Agrees with IR measurements

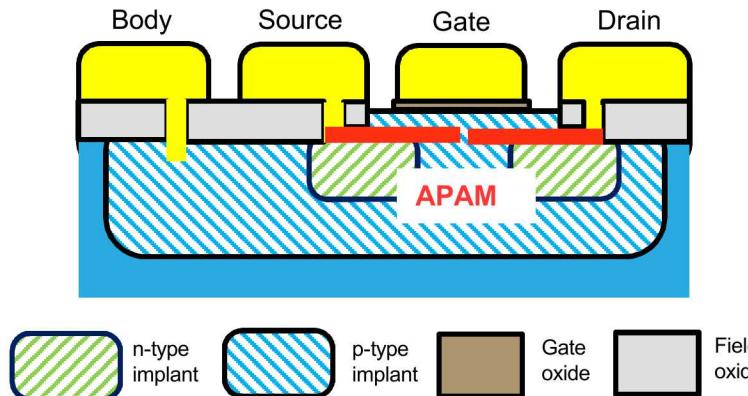
Katzenmeyer, in submission to JMR (2020)

What's next?



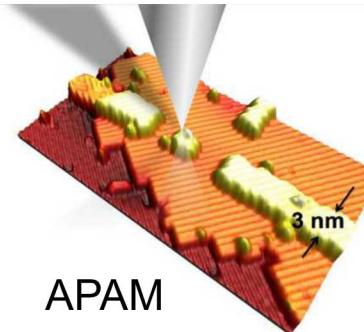
How to get to digital electronics at the atomic scale?

1. APAM devices



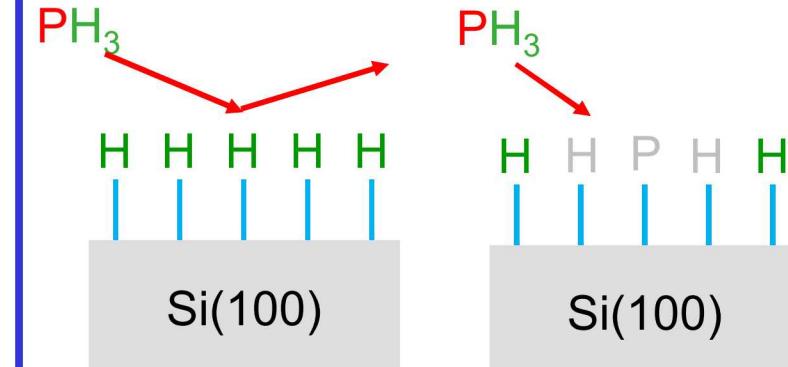
- ✓ Surface gated APAM devices
- ✓ Operate at room temperature
- ☐ APAM transistor

2. CMOS integration



- ☐ Incompatible with CMOS workflows / parts

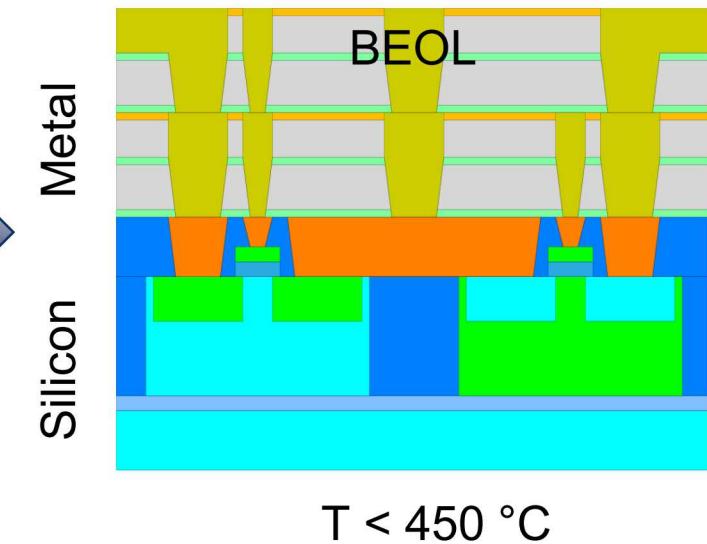
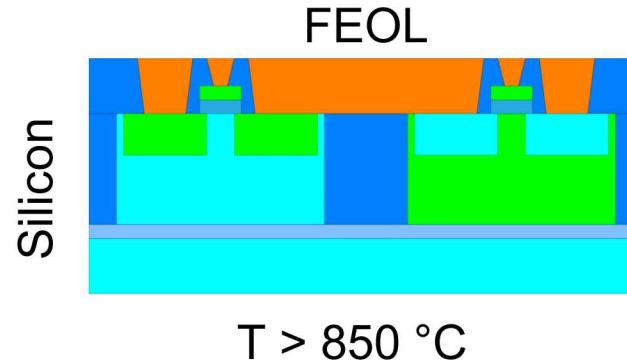
3. APAM toolkit



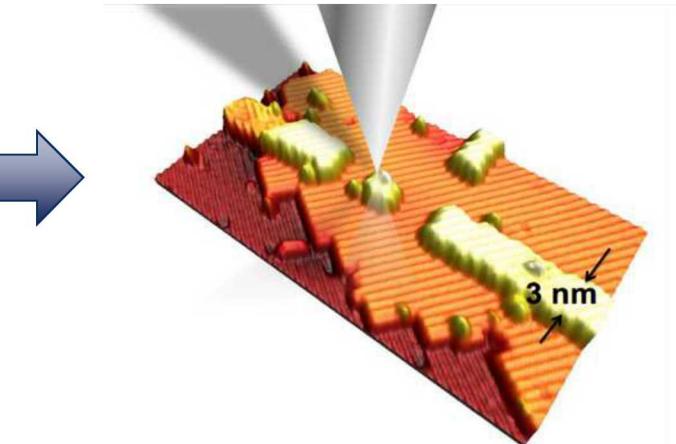
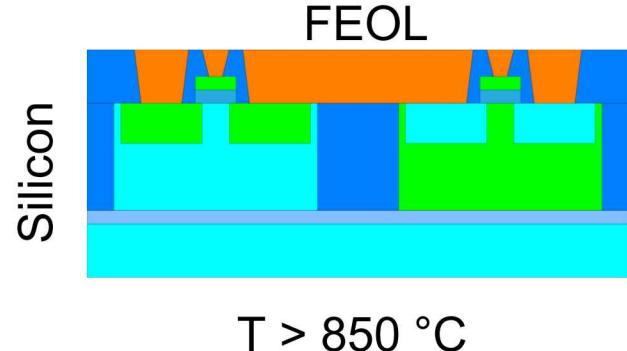
- ☐ One working chemistry

Is APAM thermally compatible with CMOS fab?

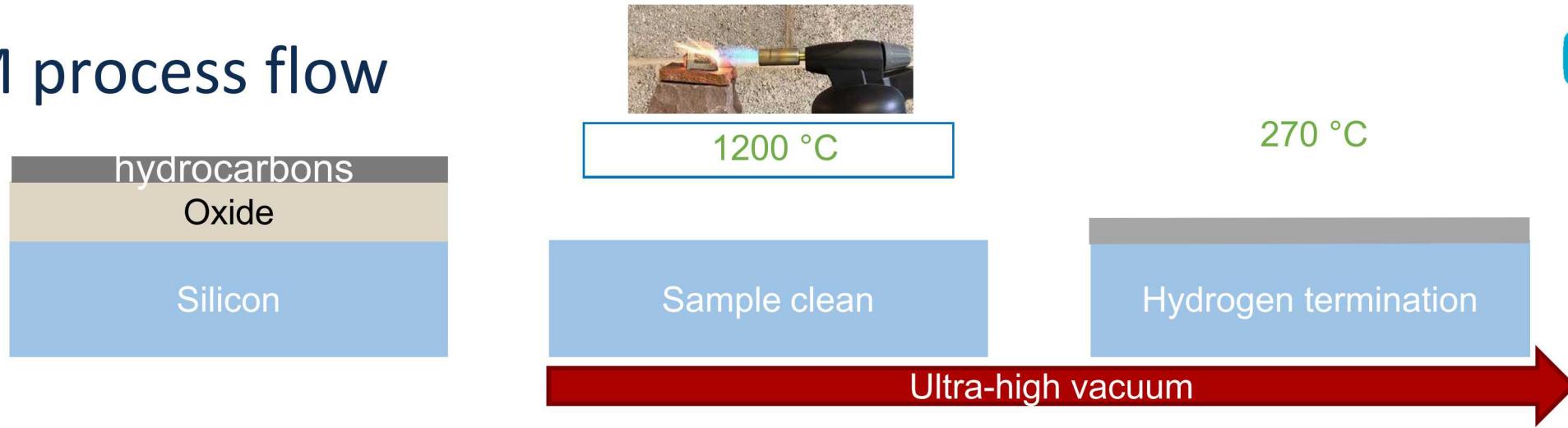
Direct CMOS Integration



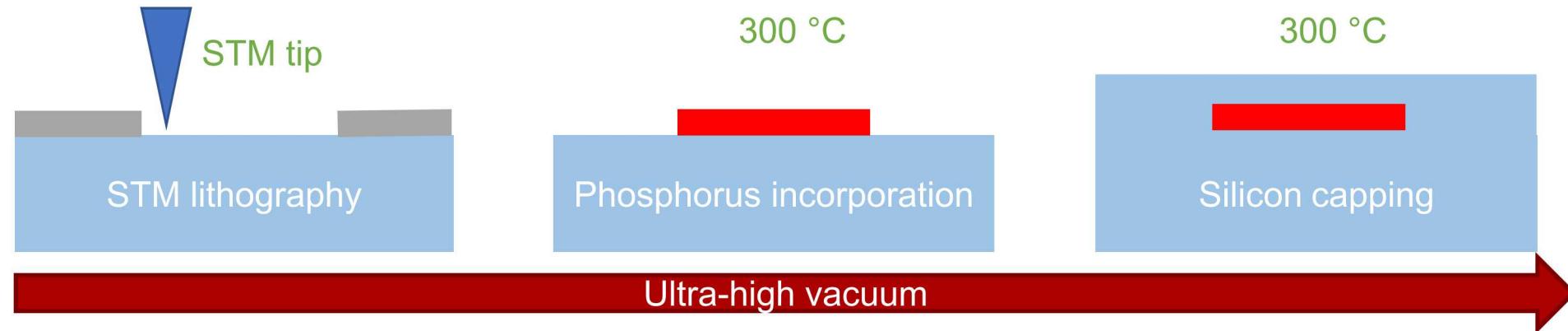
Post CMOS Integration



APAM process flow

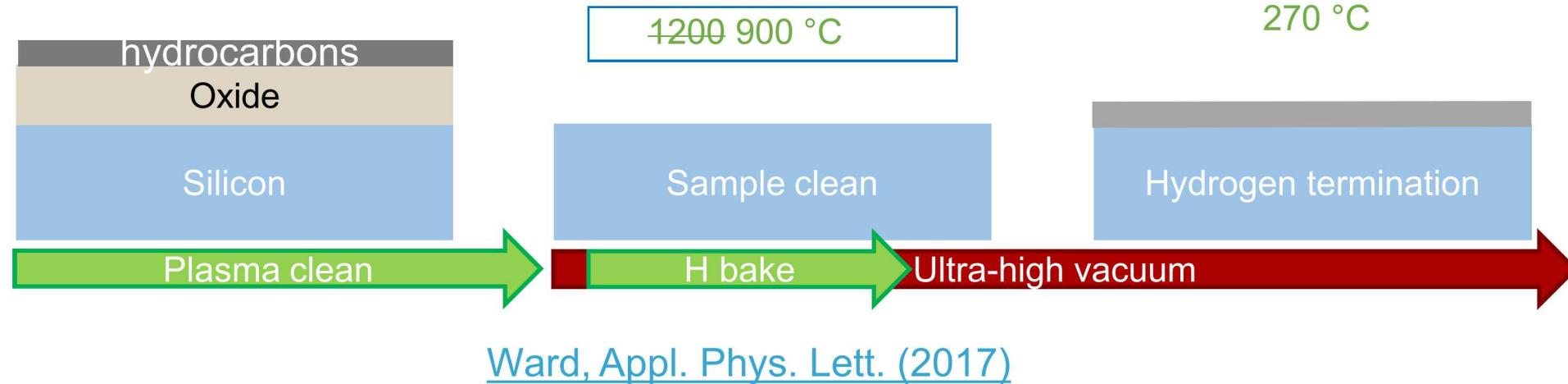


High-temperature clean destroys anything on chip before APAM.

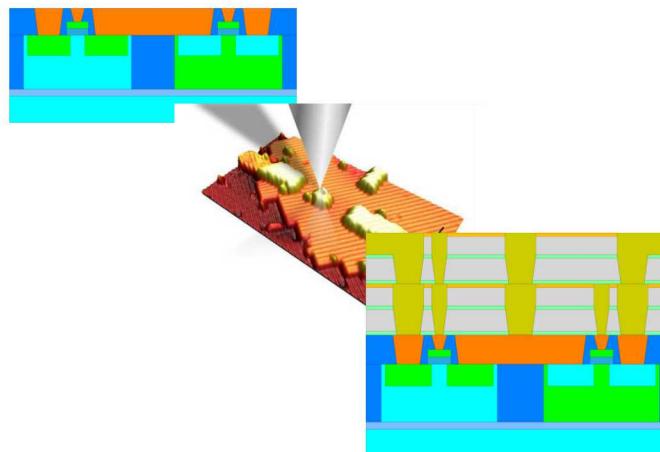


APAM will start to diffuse above 350 – 550 °C

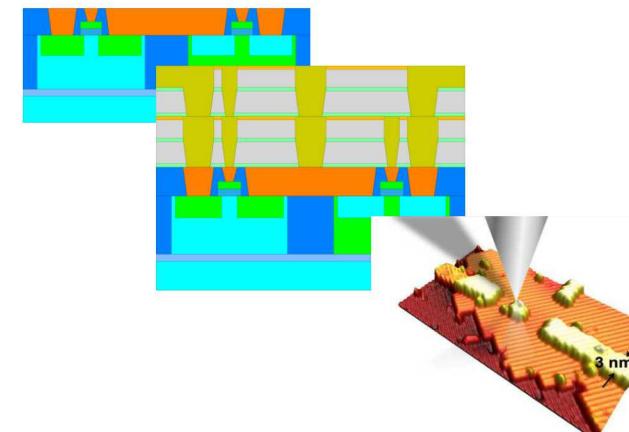
APAM process flow



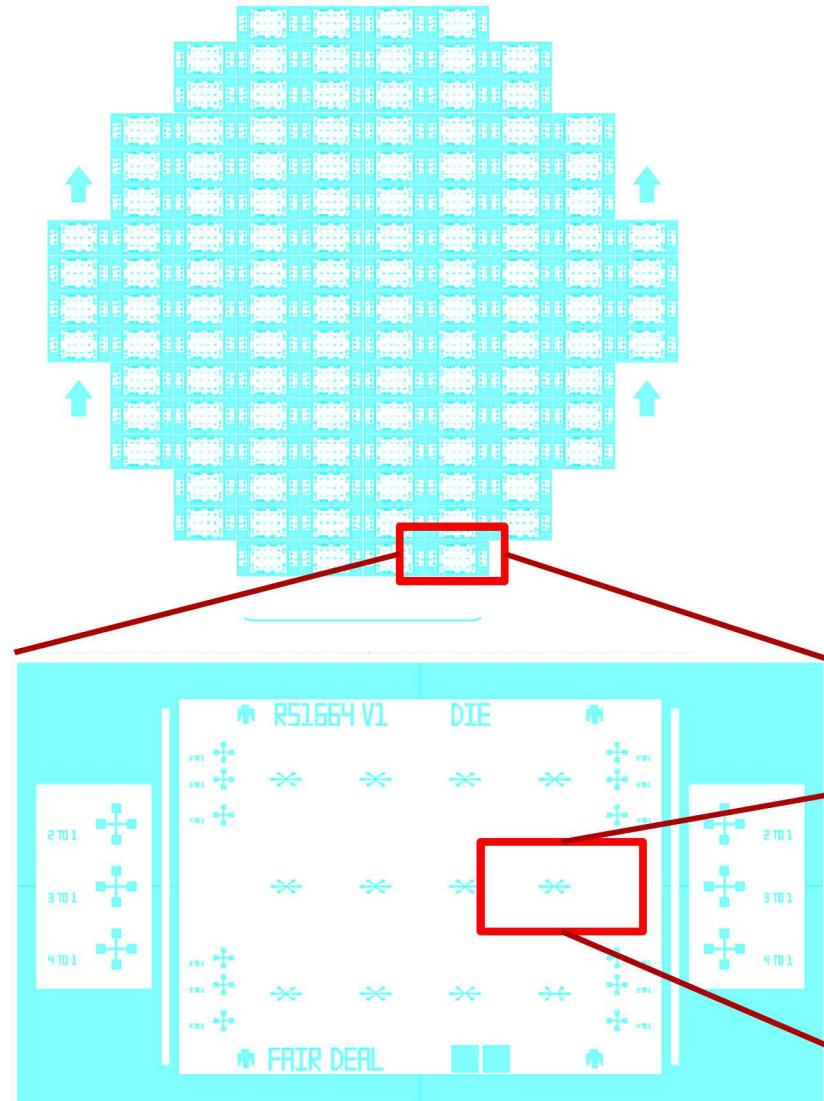
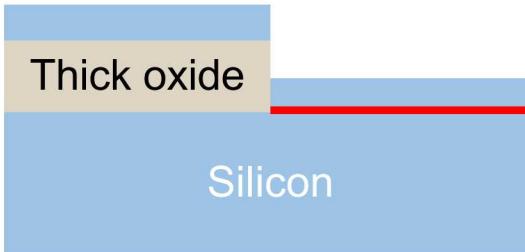
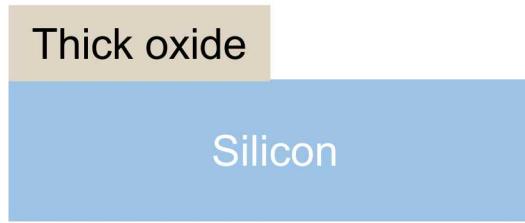
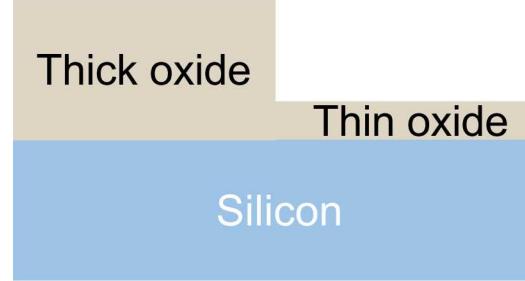
Direct Integration: can we do wafer-scale APAM processing?



Post-CMOS integration: how low can we drive down process temperatures, even with sub-optimal results?



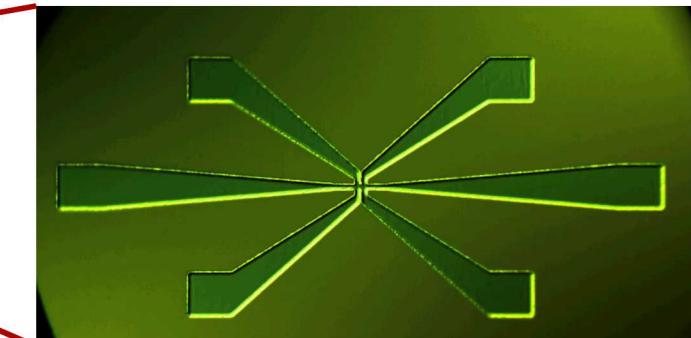
Scale APAM using hard masks



Oxide film + thermal prep works.

For CMOS integration –

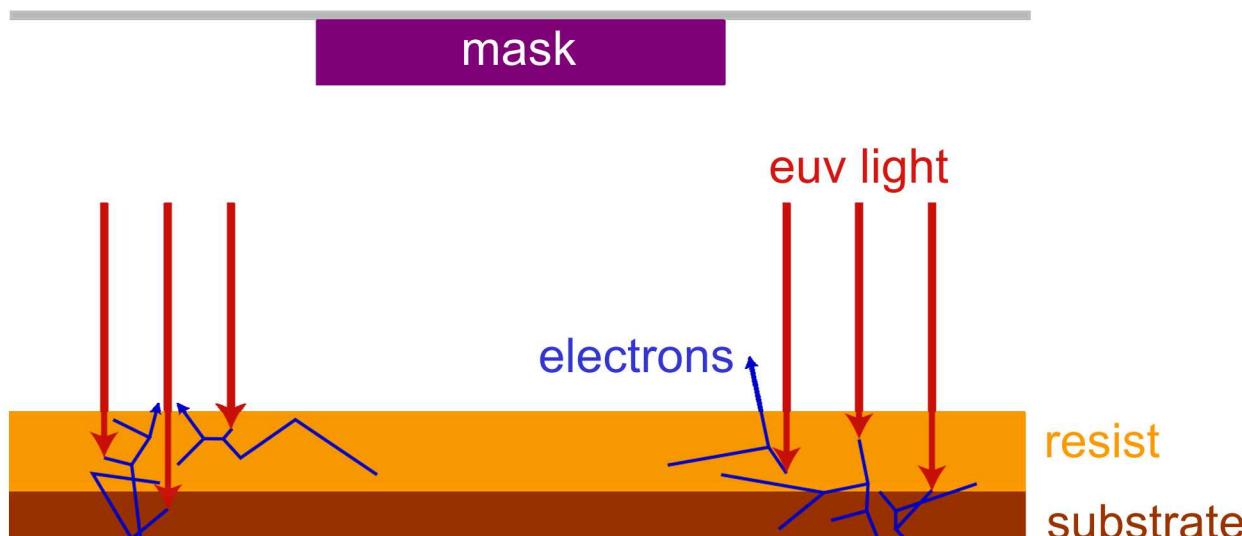
- Nitride films
- Sputter clean
- Check local interconnects survive



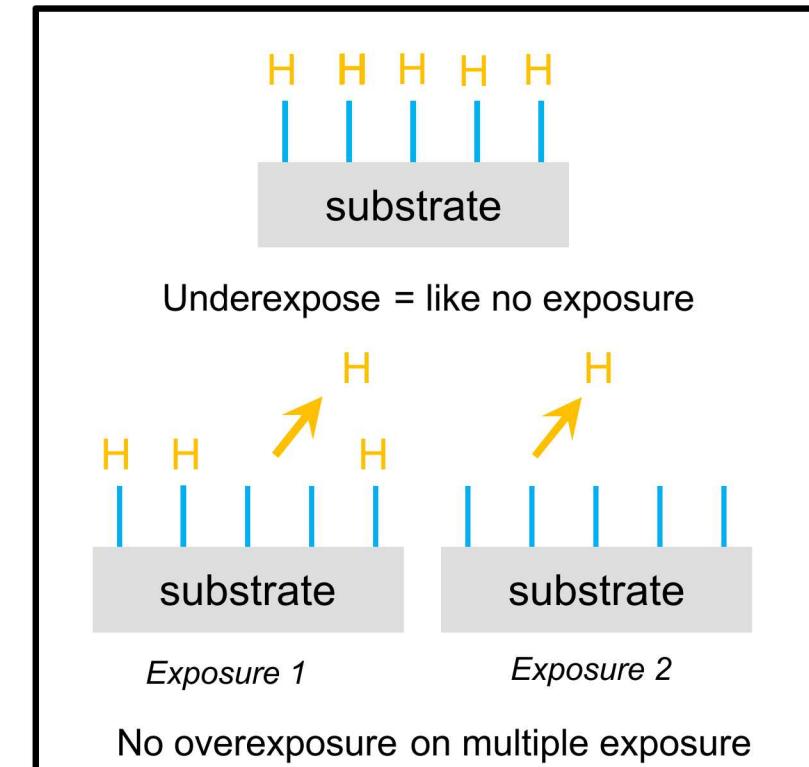
Not just 'atom-sized transistors'... atomic-scale processing

Traditional polymer resist

- Shot noise of light
- Statistics of e- generation
- Statistics of polymers



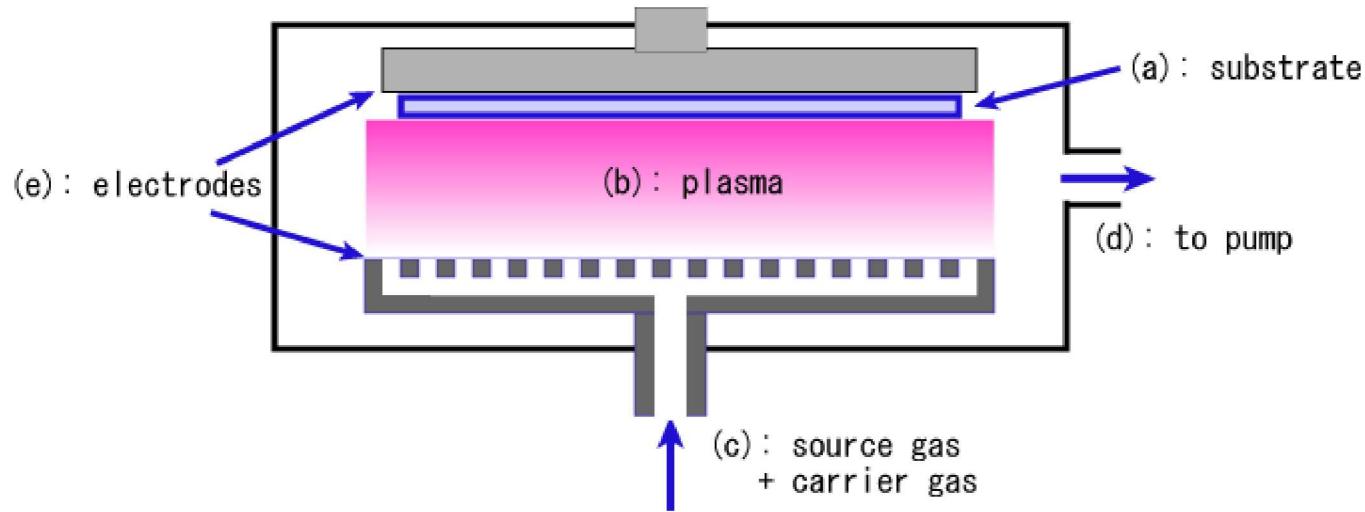
Atomic-scale resist



- Can't be over-exposed or under-exposed
→ solves problems with shot noise
- Stable to arbitrary pitch
- [Katzenmeyer, Proc. SPIE \(2020\)](#)

Scale APAM process

Wafer-scale processing by adding on to existing tool (ALD or CVD)

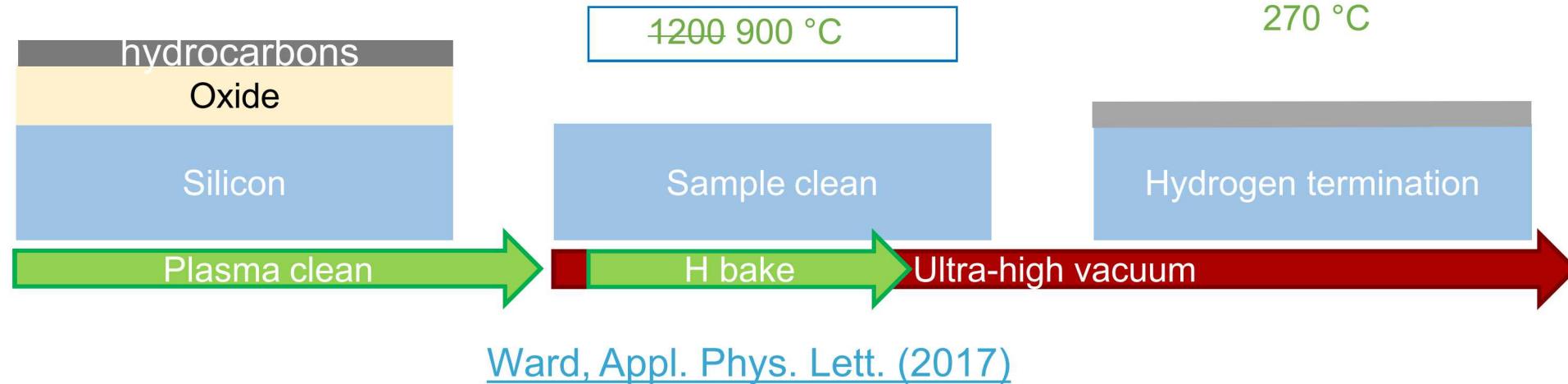


Challenges:

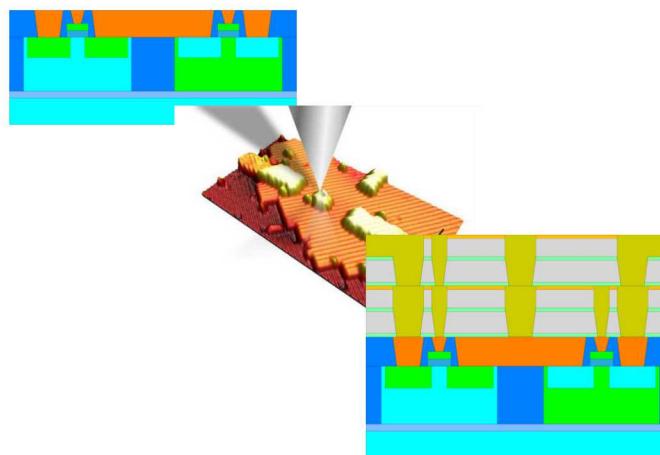
- Elevated pressure
 - After wafer clean – proceed to doping, or preserve surface with H?
 - Kinetics of dopant incorporation
- Low temperature growth
 - Only MBE known to work at these temperatures
 - Radical growth? Beam-assisted? Chemical - TCS/DS?

Looking for partners.
Skywater Technologies can host a tool.

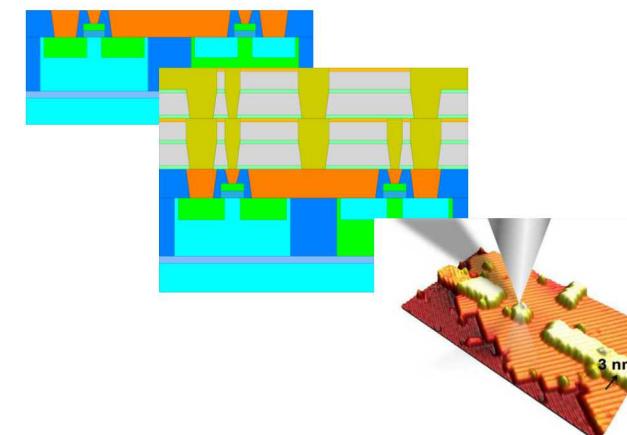
APAM process flow



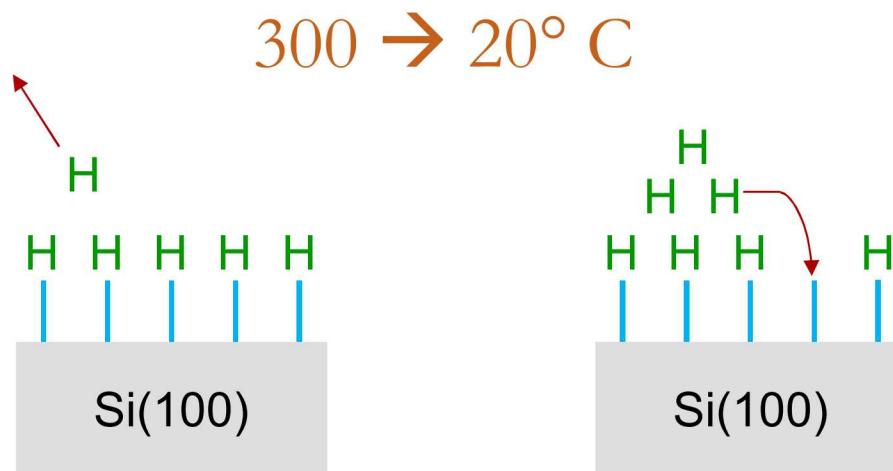
Direct Integration: can we do wafer-scale APAM processing?



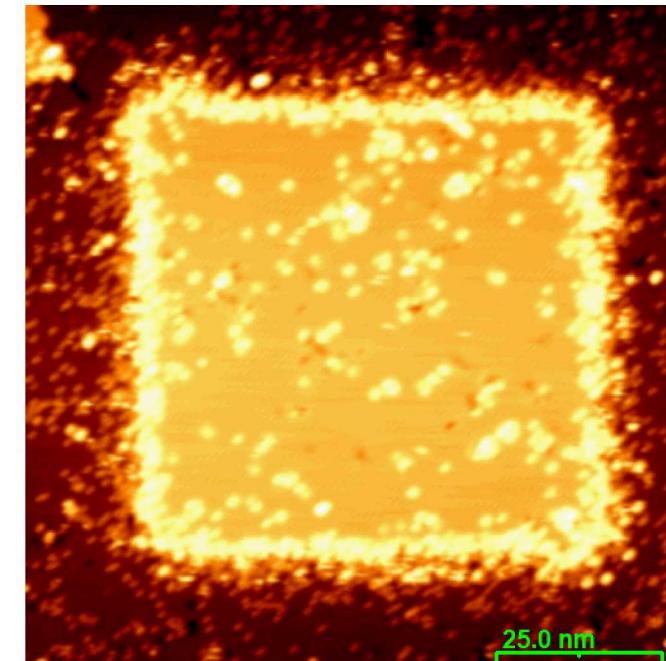
Post-CMOS integration: how low can we drive down process temperatures, even with sub-optimal results?



Hydrogen passivation & lithography



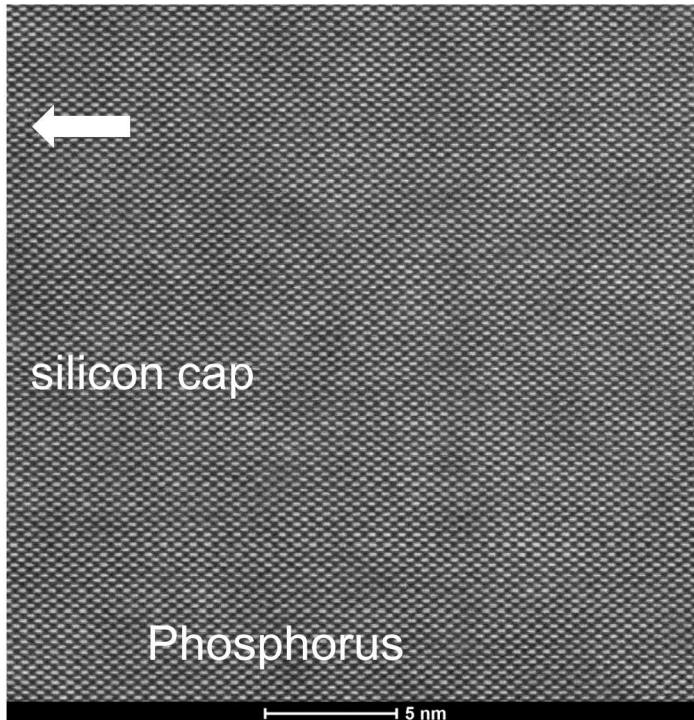
20° C: Hydrogen physisorbed on top of hydrogen passivated silicon



Lithography now requires multiple passes, but works great!

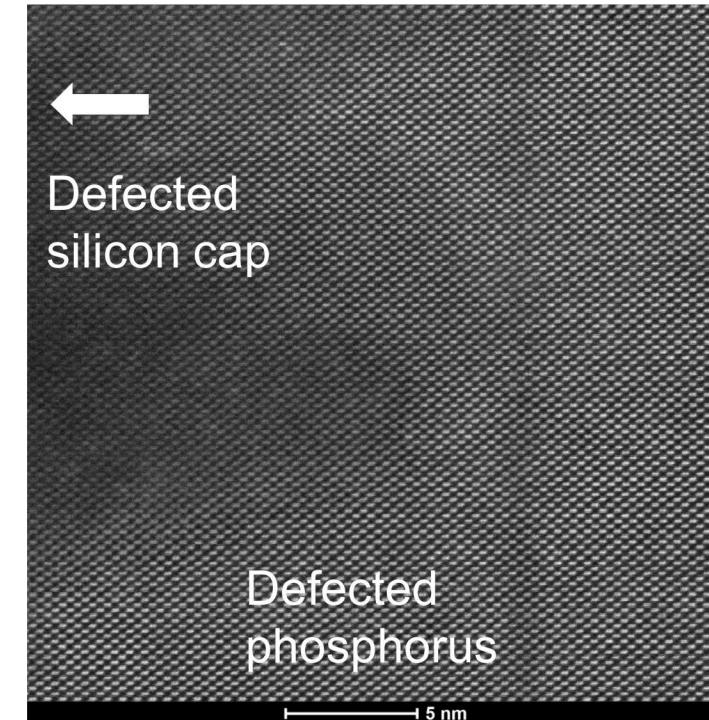
Phosphorus incorporation and capping

$350 \rightarrow 200^\circ \text{ C}$



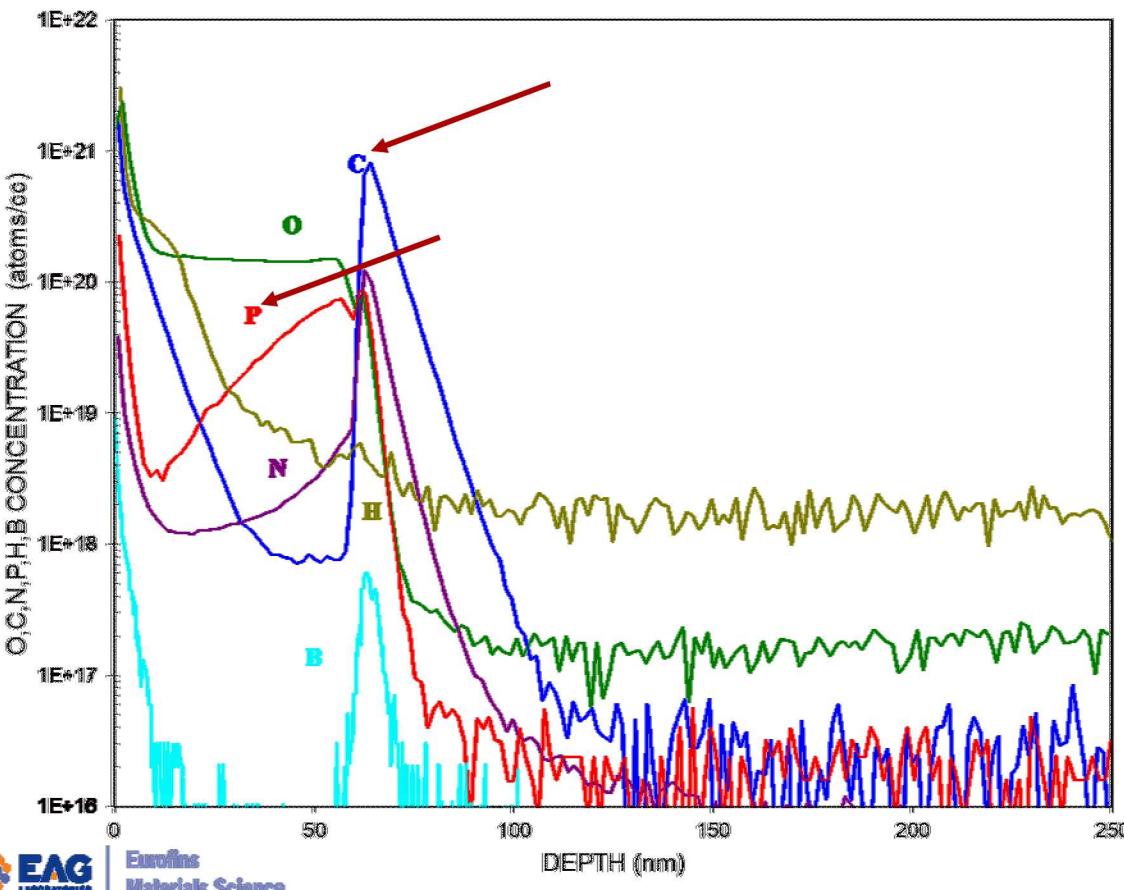
$n \sim 1.7 \times 10^{14} \text{ cm}^{-2}$
 $\mu \sim 50 \text{ cm}^2/\text{V-s}$
 $\sigma \sim 2 \text{ mS/sq.}$

Electrical transport
degrades only by a factor
of 3 vs. optimal process



$n \sim 1.4 \times 10^{14} \text{ cm}^{-2}$
 $\mu \sim 20 \text{ cm}^2/\text{V-s}$
 $\sigma \sim 0.6 \text{ mS/sq.}$

Reduced temperature sample prep

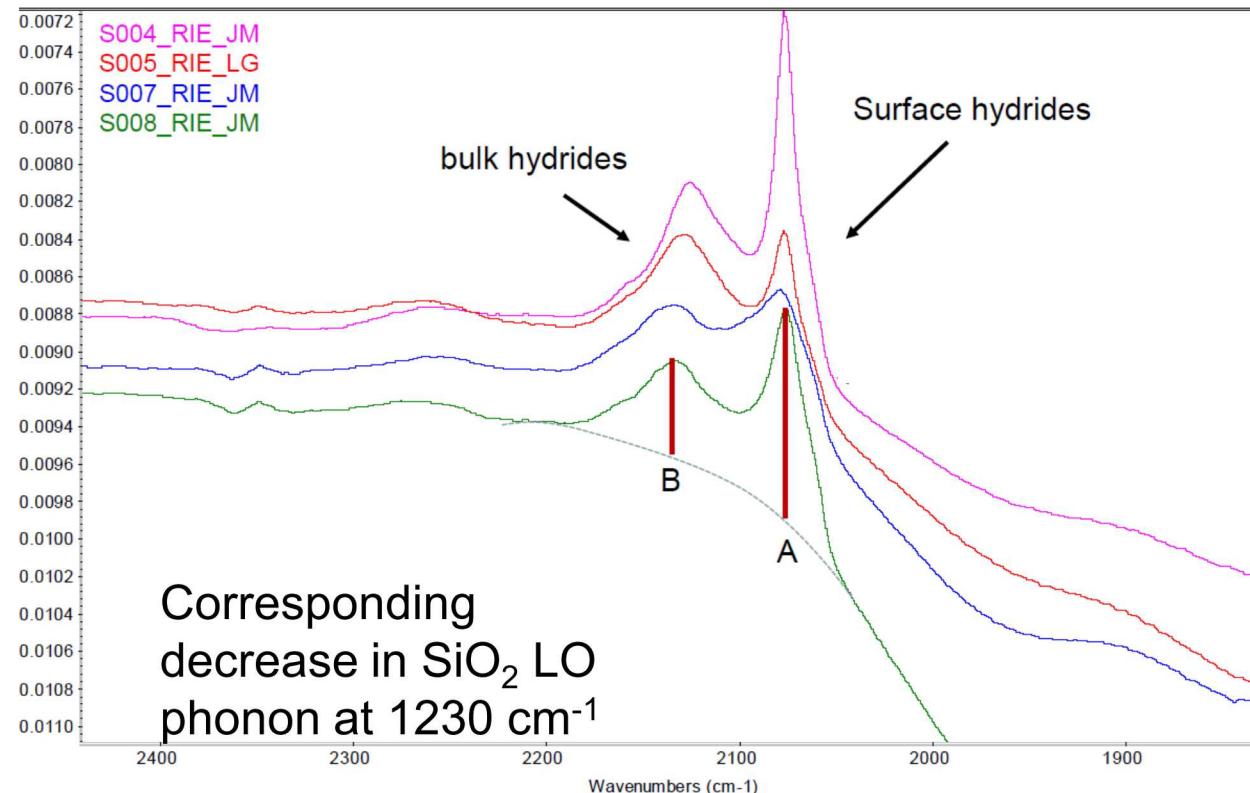


 **EAG** Materials Science

Wet preparation is not working

Hines, *J. Phys. Chem. C* (2009)

IR differential spectra of hydrogen stretch region

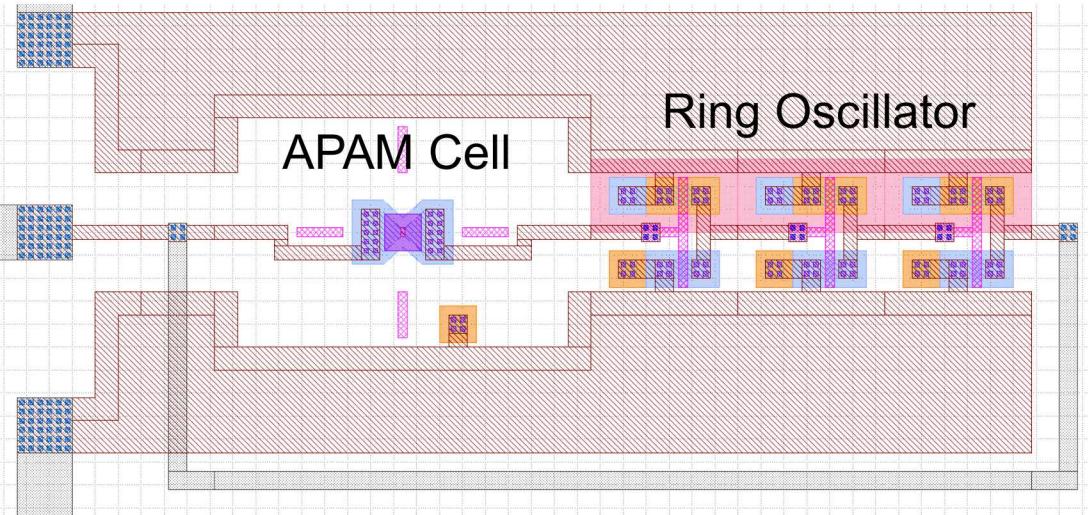


Corresponding decrease in SiO_2 LO phonon at 1230 cm^{-1}

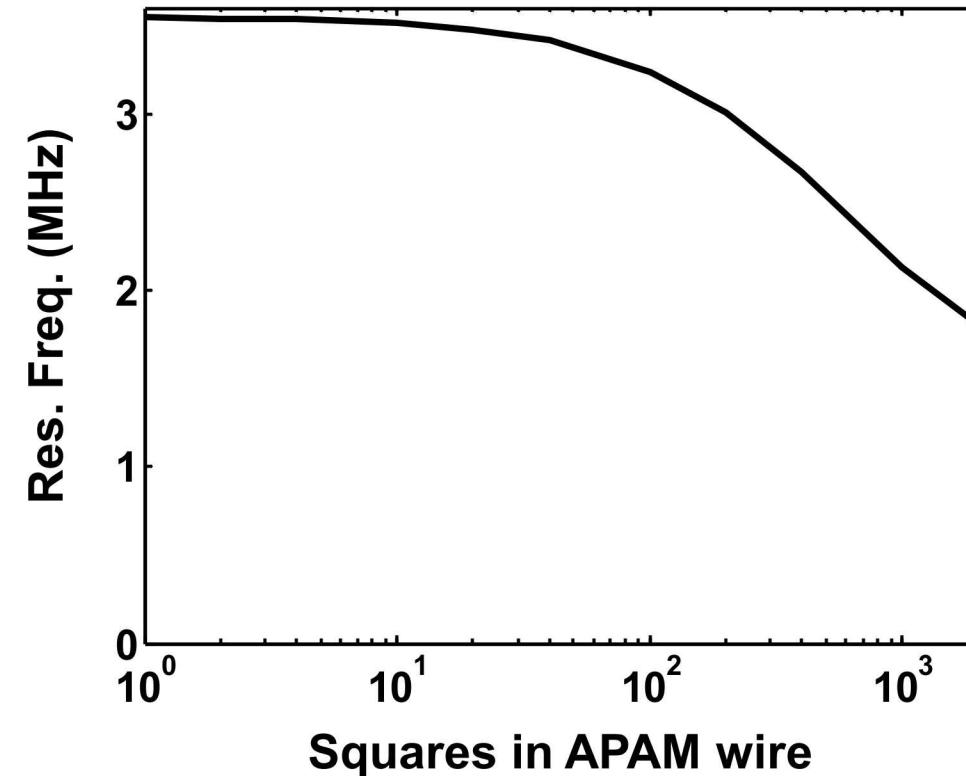
RIE has shown promising results, but reproducibility problems. Trying in a variety of tools.

What's next? Go for it!

Physical Layout



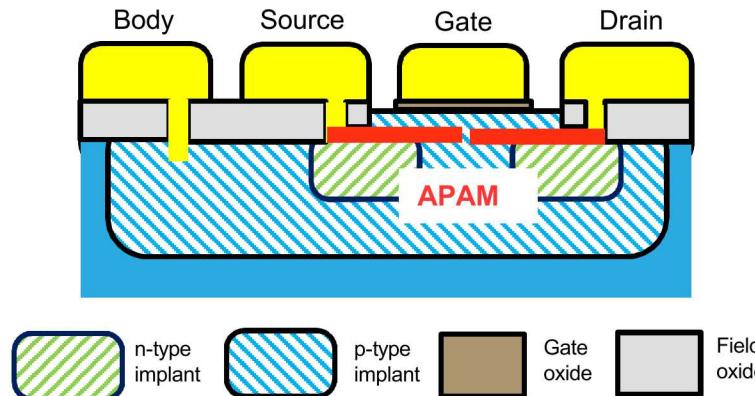
Full-stack simulation



Measure effect of APAM on real CMOS parts

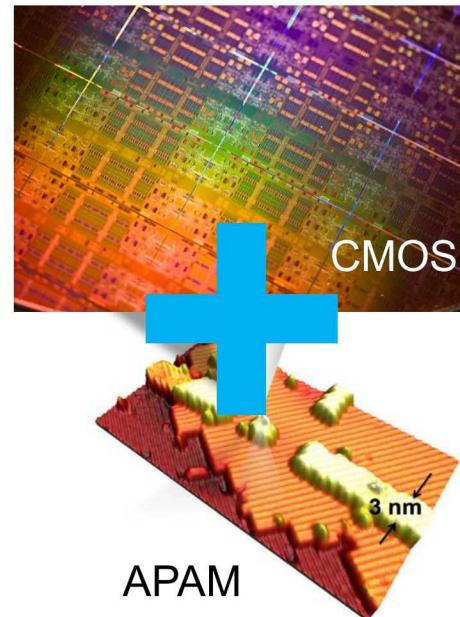
How to get to digital electronics at the atomic scale?

1. APAM devices



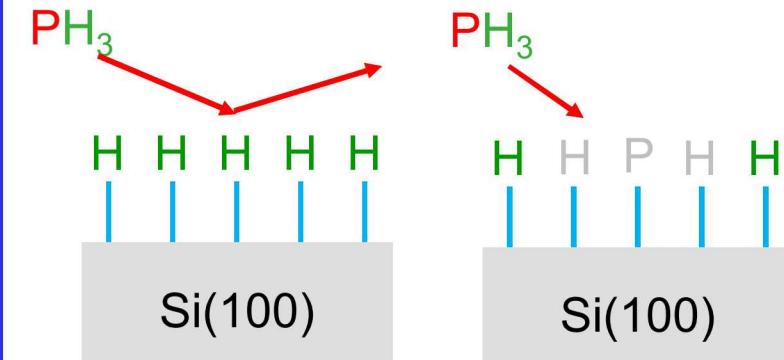
- ✓ Surface gated APAM devices
- ✓ Operate at room temperature
- ☐ APAM transistor

2. CMOS integration



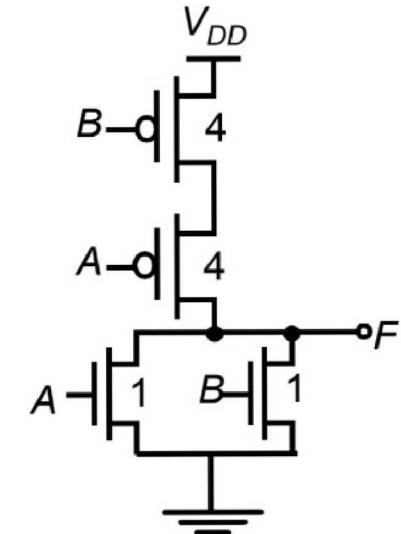
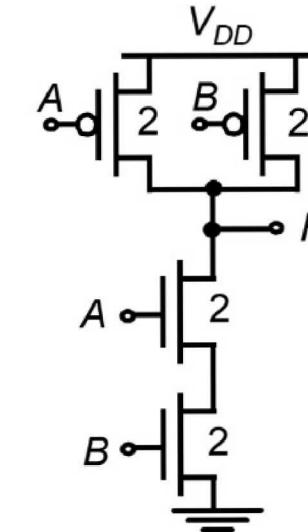
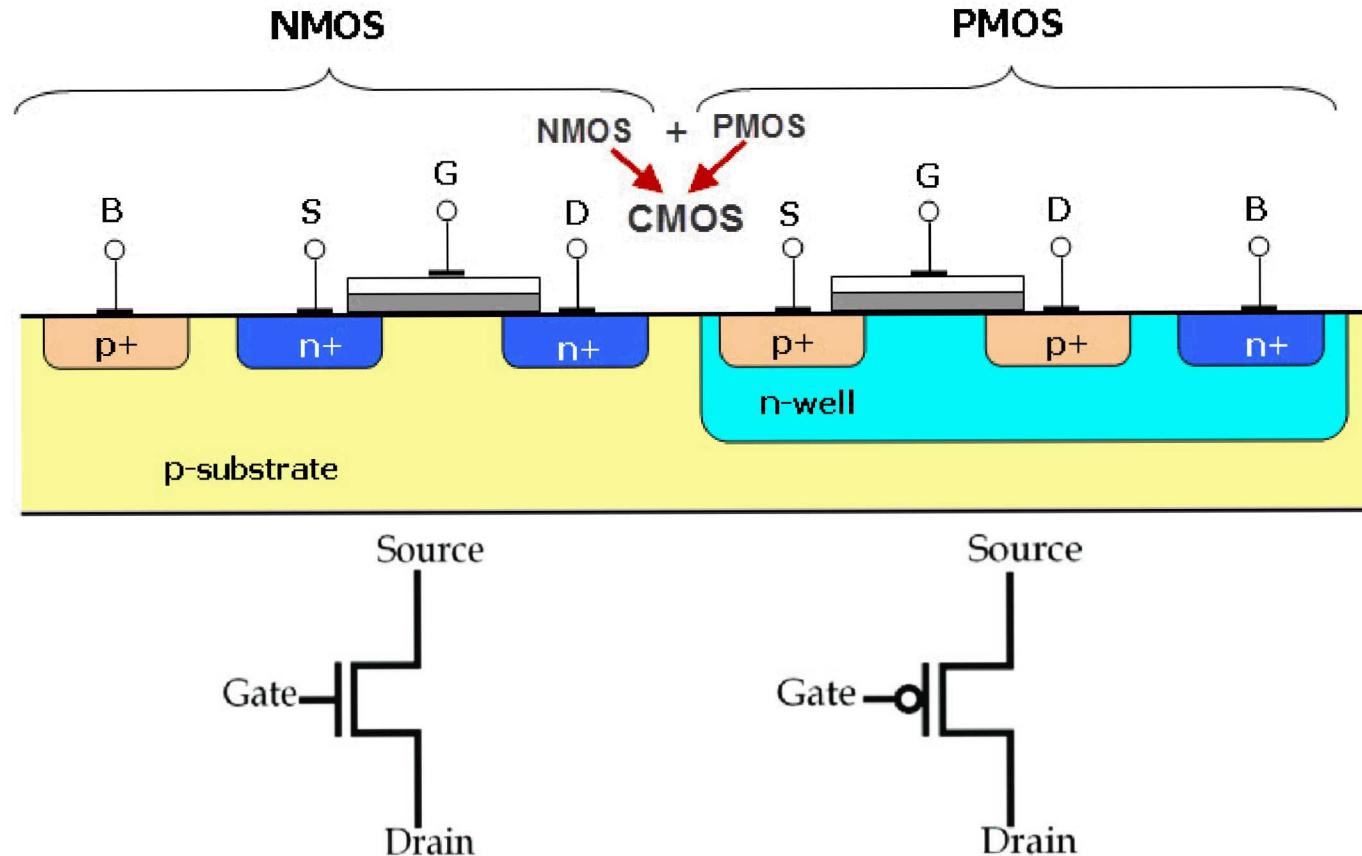
- ✓ Direct integration: wafer-scale APAM litho
- ☐ Wafer-scale APAM process
- ✓ Post-CMOS: reduction of process temperatures
- ☐ Reduced temp. sample prep

3. APAM toolkit



- ☐ One working chemistry

Need an acceptor chemistry

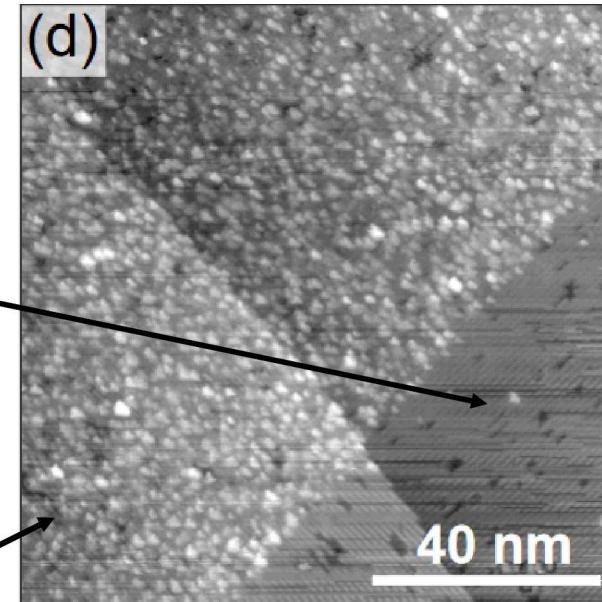
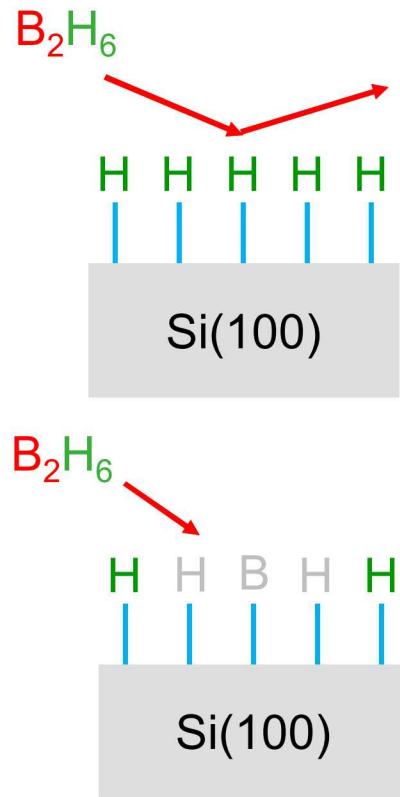


Efficient digital logic requires complementary switches

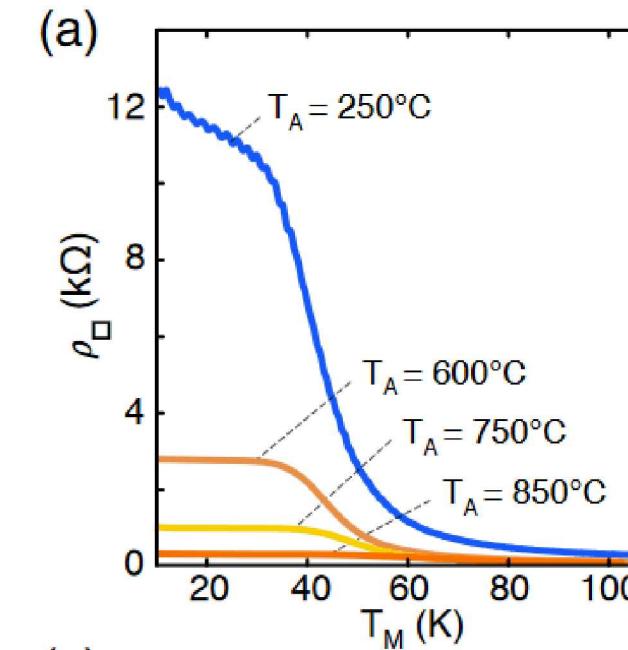
Complementary devices require acceptors.

Diborane provides selective p-type doping

Skeren, arXiv:1912.06188

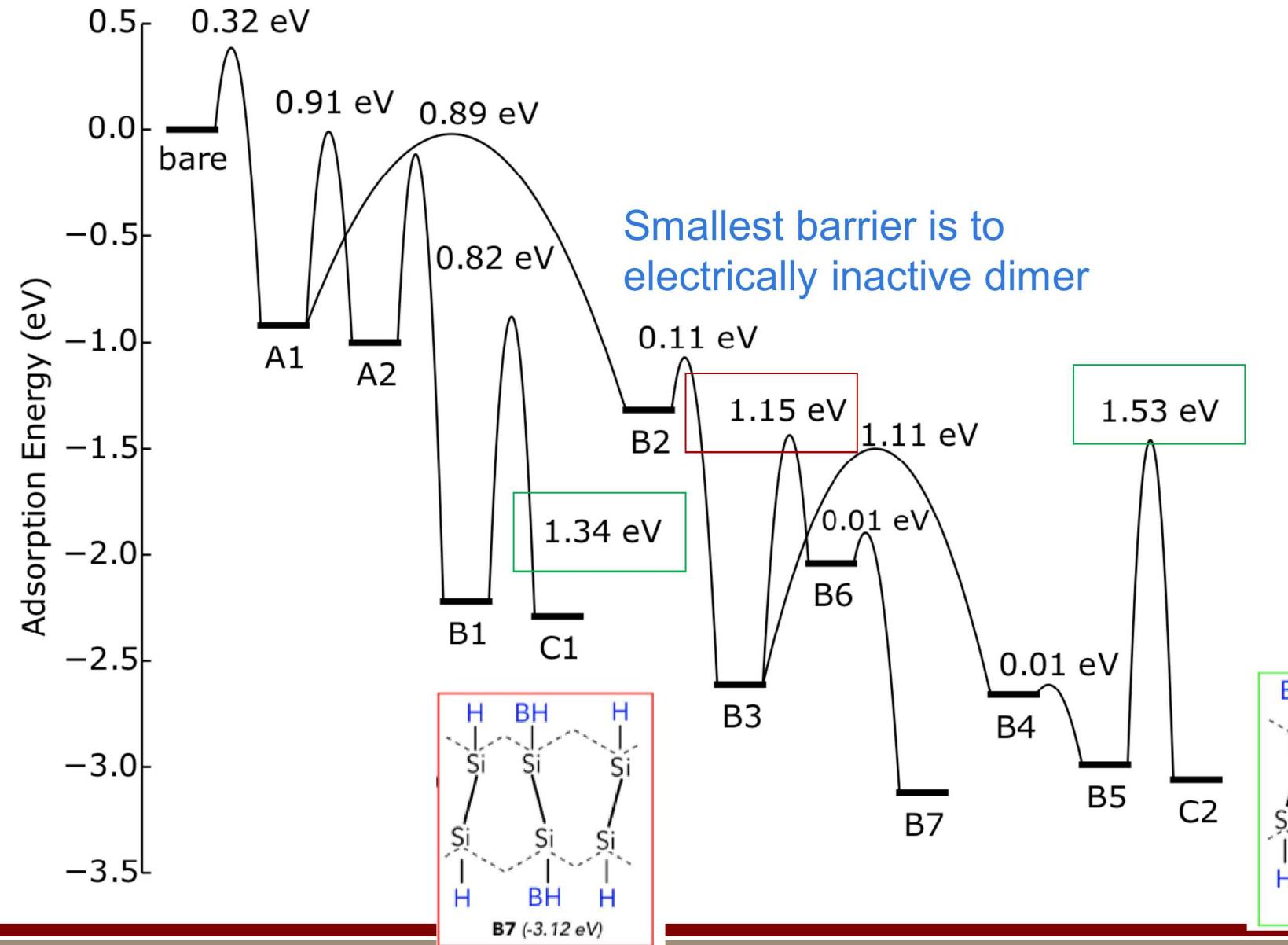
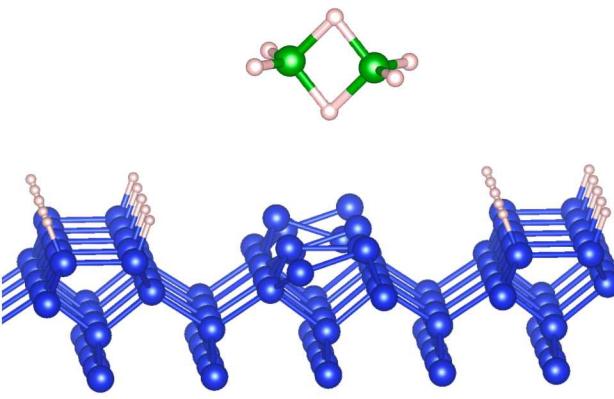


B_2H_6 sticks selectively!

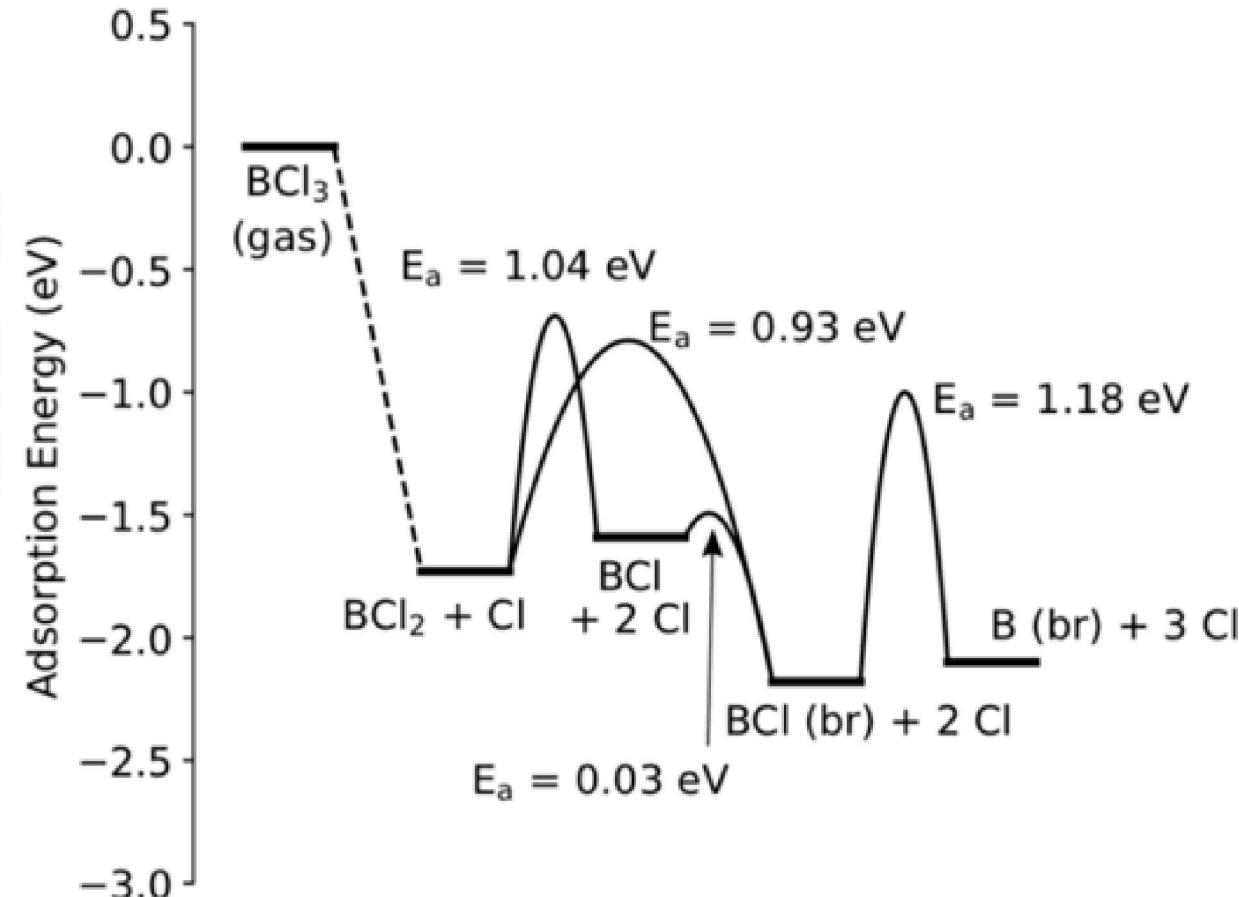
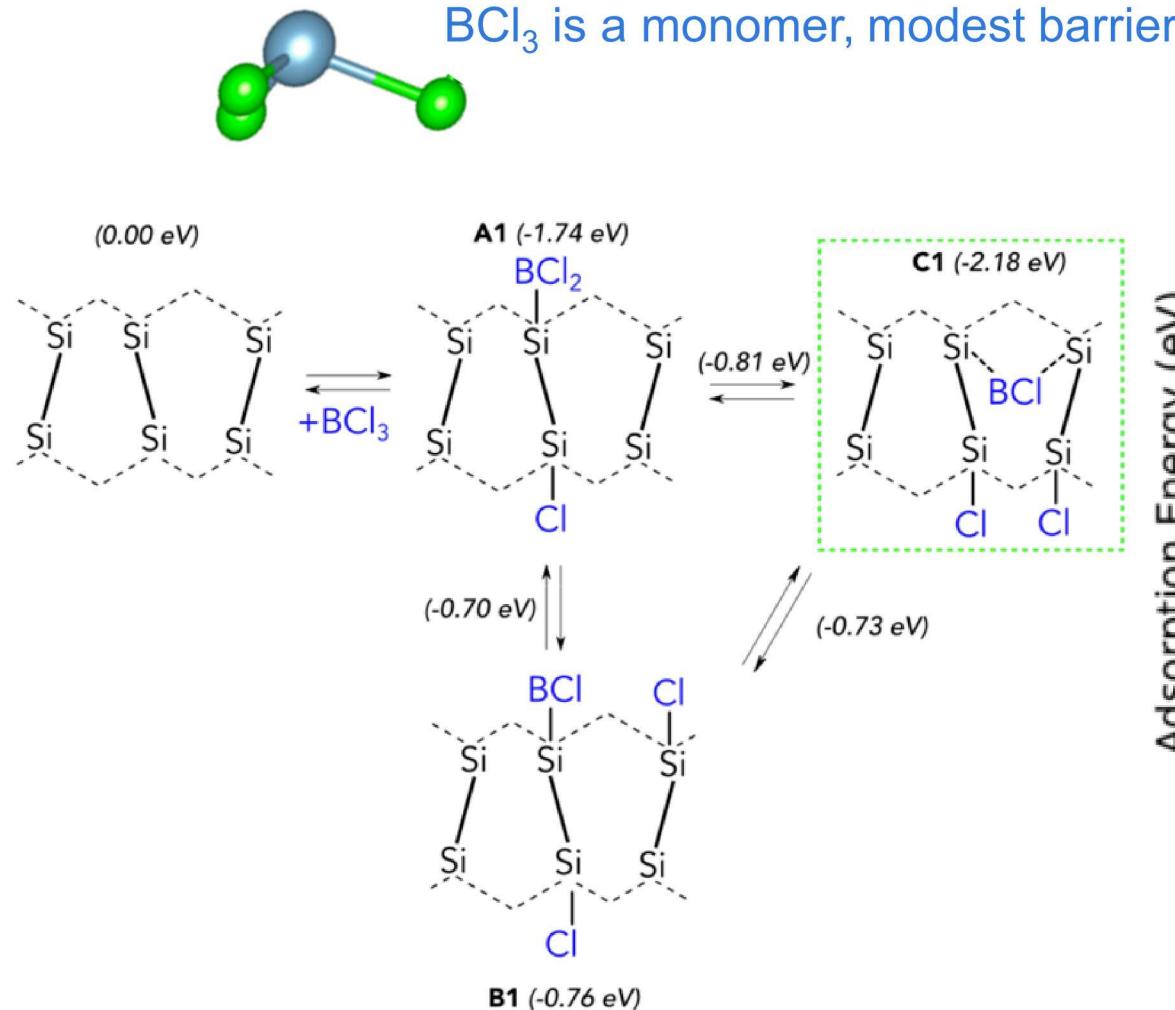


Electrical quality is questionable

Why does diborane have a high resistivity?

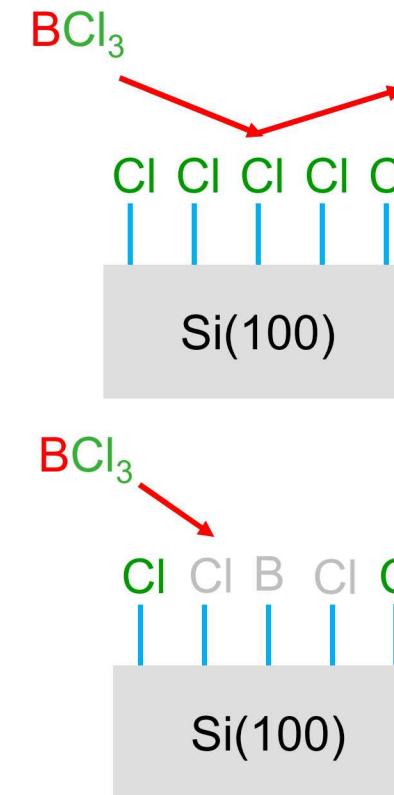
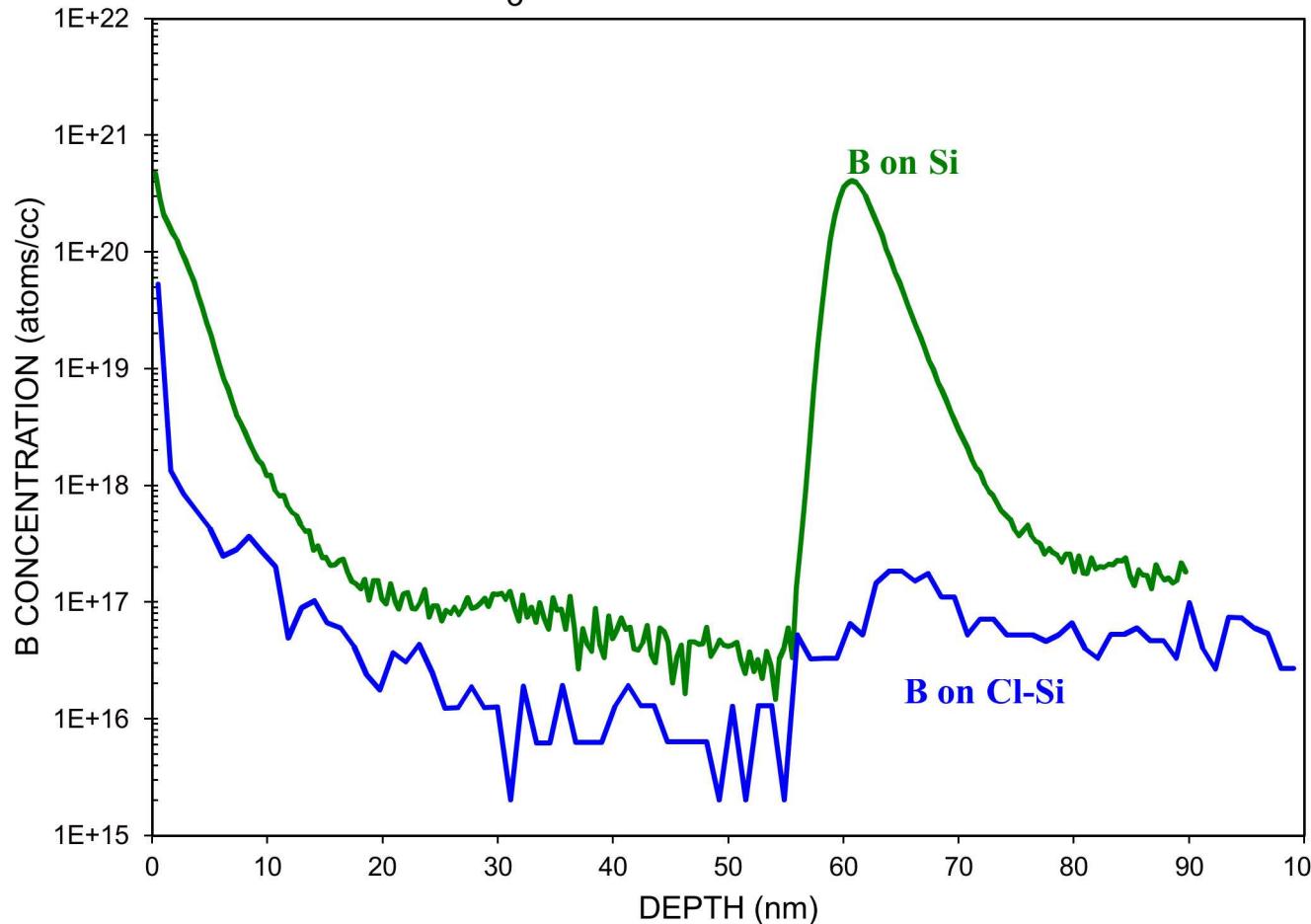


Acceptor chemistry with monomer precursor

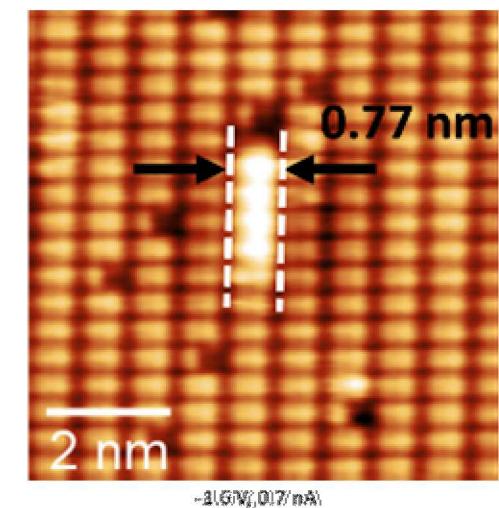


BCl_3 selective to Cl/bare silicon

3.6 L BCl_3 on bare and Cl-terminated Si

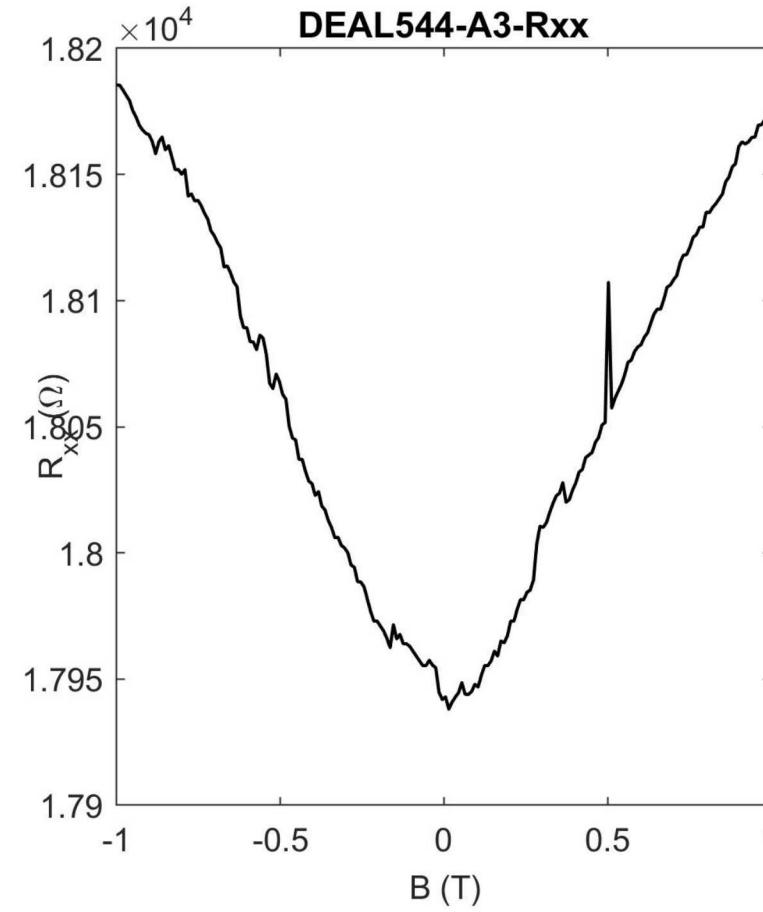
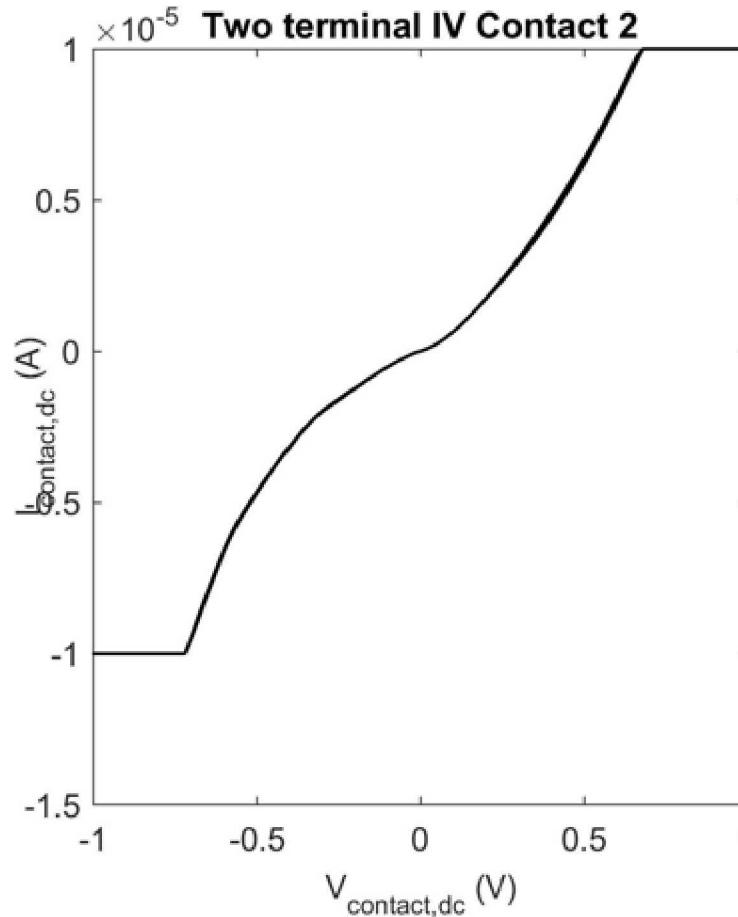


Atomic Precision
Patterning



[Dwyer, J. Phys. Chem. A \(2019\)](#)

First electrical measurements

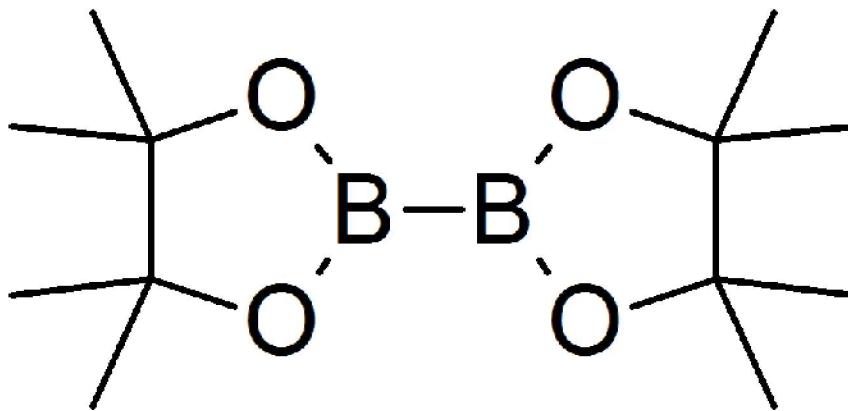


Resistivity of $2.25 \text{ k}\Omega/\text{sq}$

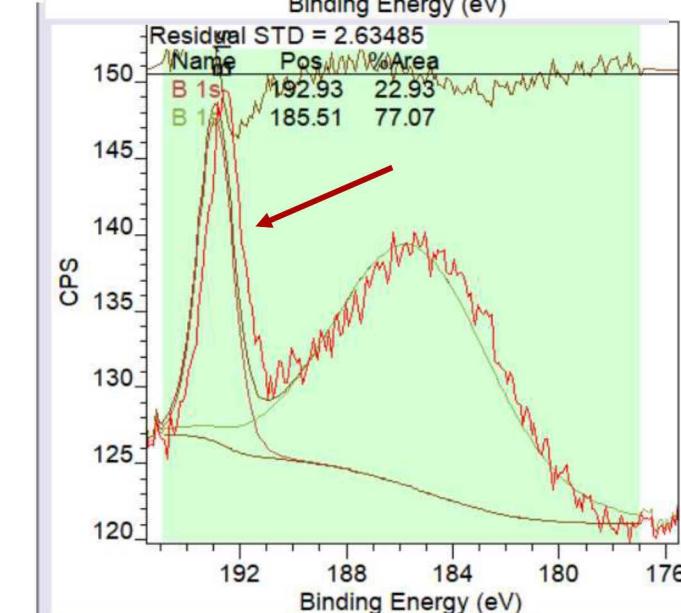
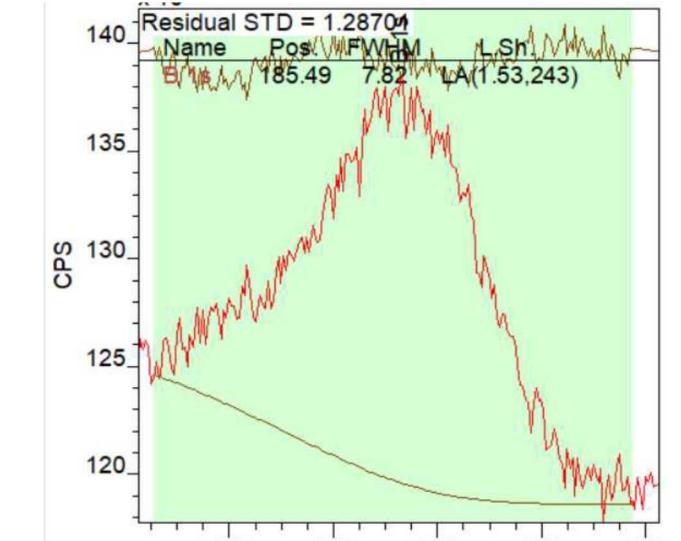
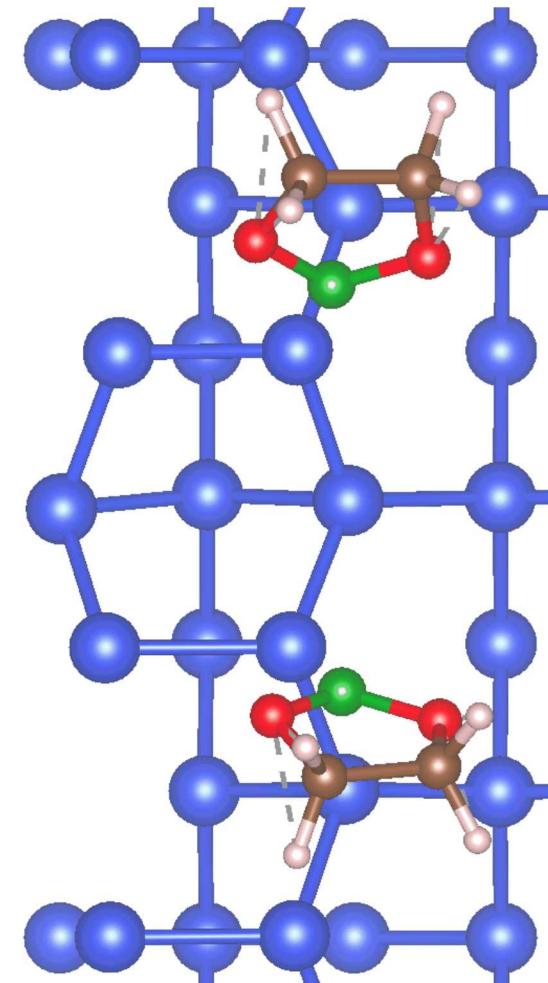
- 4x worse than phosphine
- 6x better than diborane

What's next?

Need wider range of chemistries,
but hard to try... try wet chemistry

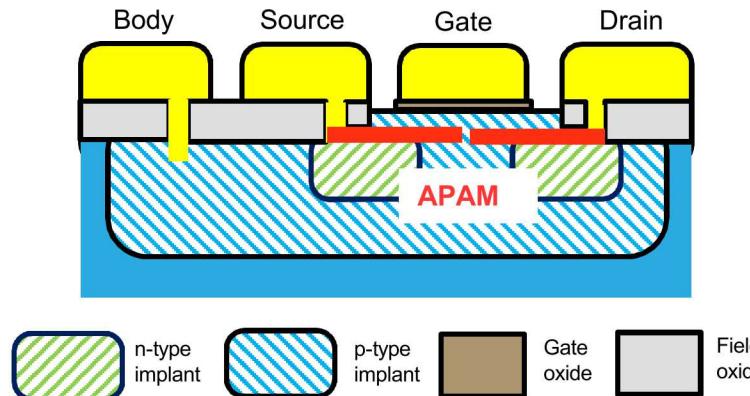


How do people clean up
wet chemistry?



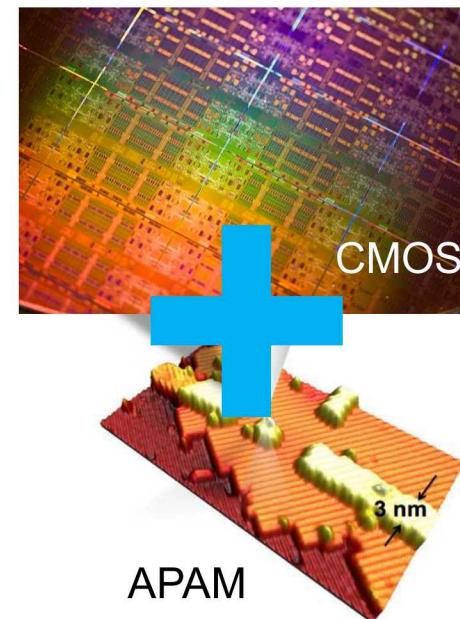
How to get to digital electronics at the atomic scale?

1. APAM devices



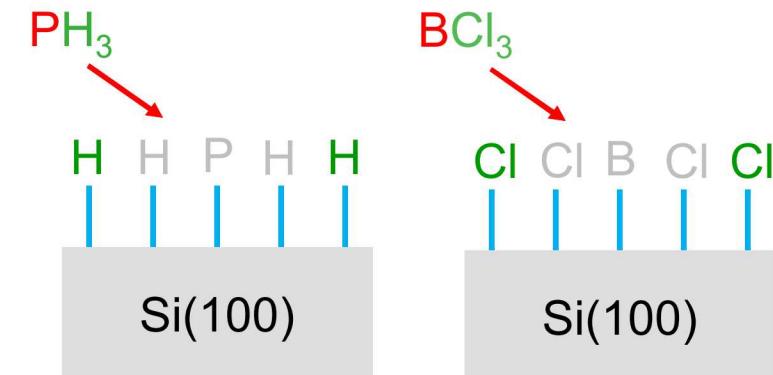
- ✓ Surface gated APAM devices
- ✓ Operate at room temperature
- ❑ APAM transistor

2. CMOS integration



- ✓ Direct integration: wafer-scale APAM litho
- ❑ Wafer-scale APAM process
- ❑ Post-CMOS: Reduced temp. sample prep

3. APAM toolkit



- ✓ Working chemistry with PH_3 / H and BCl_3 / Cl
- ❑ Chemistries for oxides, metal, etching, etc.

Thanks to...

Devices

Lead: Shashank Misra

Modeling

Lead: Suzey Gao

Integration

Lead: David Scrymgeour

Manufacturability

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: Bob Butera (LPS), Kevin Dwyer (LPS), Andrew Teplyakov (Delaware), Alex Shestopalov (Rochester), Ezra Bussmann, Scott Schmucker, Evan Anderson, Joe Lucero, Jeff Ivie, Fabian Pena, Aaron Katzenmeyer, George Wang, Esther Frederick, Igor Kolesnichenko, David Wheeler, Mike Marshall

Some of this work is supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories, and was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-mission 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-NA-0003525