SAND2021-2467C

Sandia National Laboratories

A chemical model for atomic-precision single-donor incorporation of phosphorus atoms in Si(100)-2x1

APS March Meeting
March 16, 2021

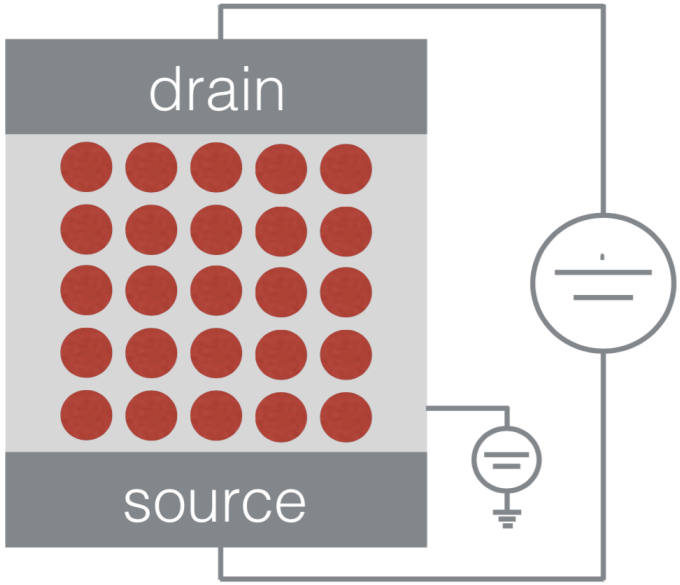
Quinn Campbell, *Jeffrey Ivie, Justin Koepke, Mitchell Brickson, Peter Schultz, Richard Muller, Ezra Bussmann, Andrew Baczewski, Andrew Mounce, Shashank Misra*

Sandia National Laboratories

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & 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.

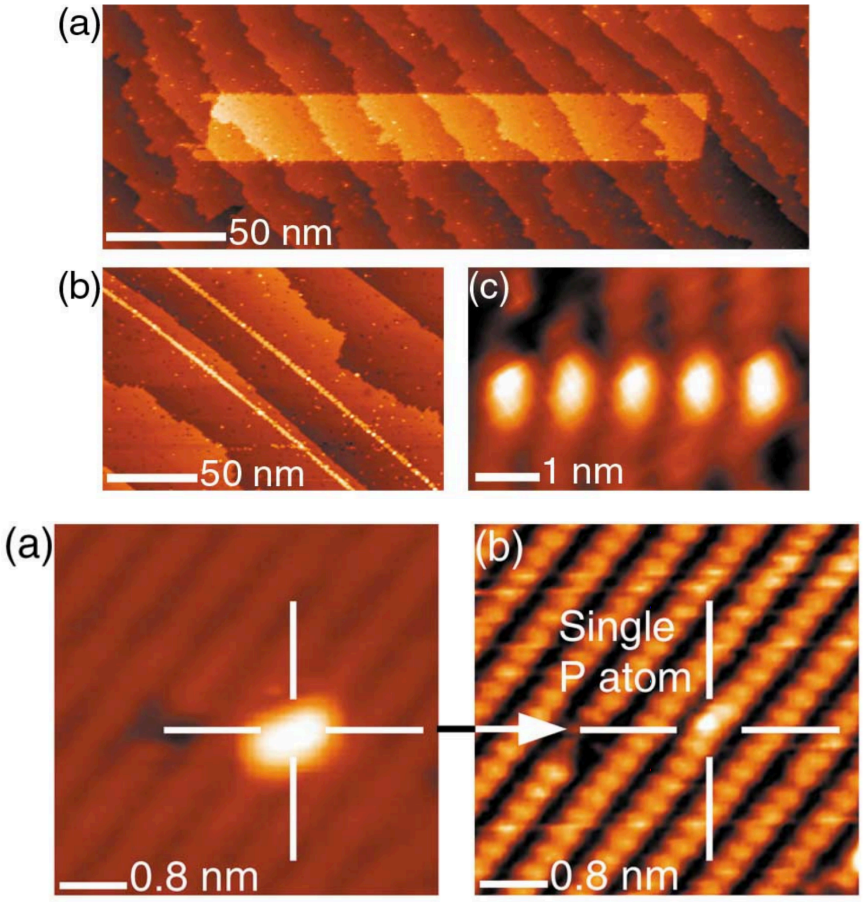
Designer quantum materials

What we would like



A controllable array of donors

What has been done

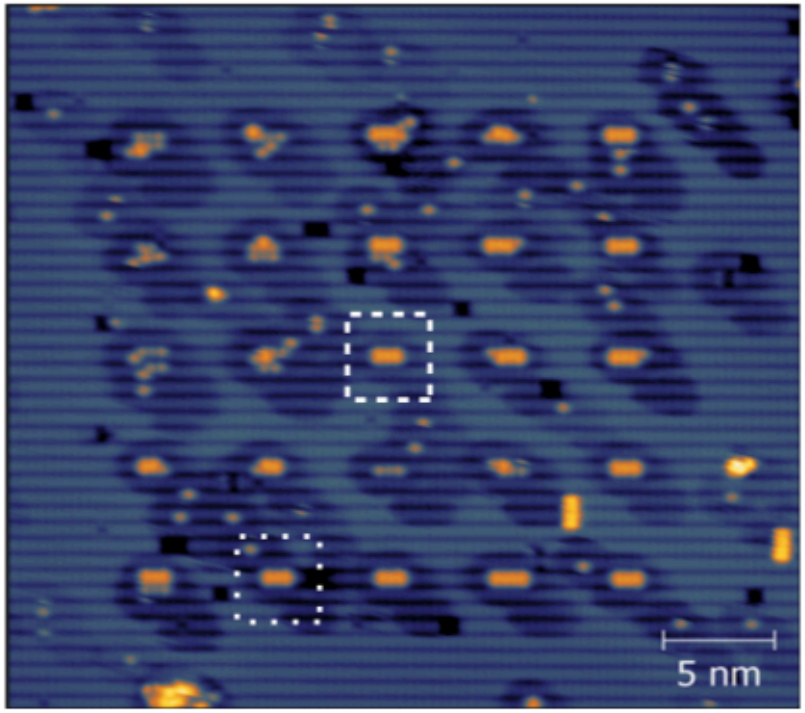


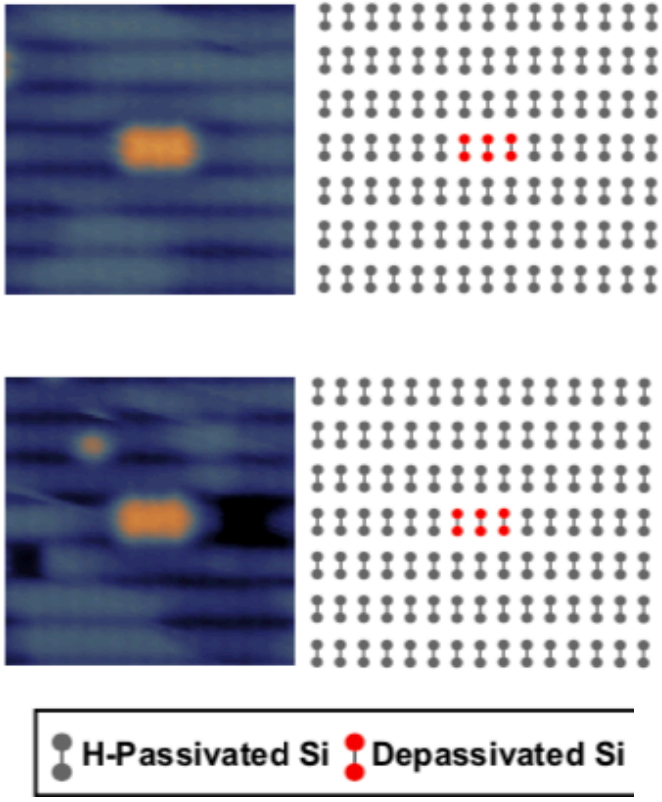
Use STM to remove a Hydrogen resist and then dose with Phosphine gas. Three silicon dimer wide windows can produce single P atom incorporation

Schofield et al., *Phys. Rev. Lett.*, **91**, 13 (2003).

Three dimer wide lithography rate

$$P(N) = \left(\sum_{w} P_L(w) P_I(n = 1|w) \right)^N$$

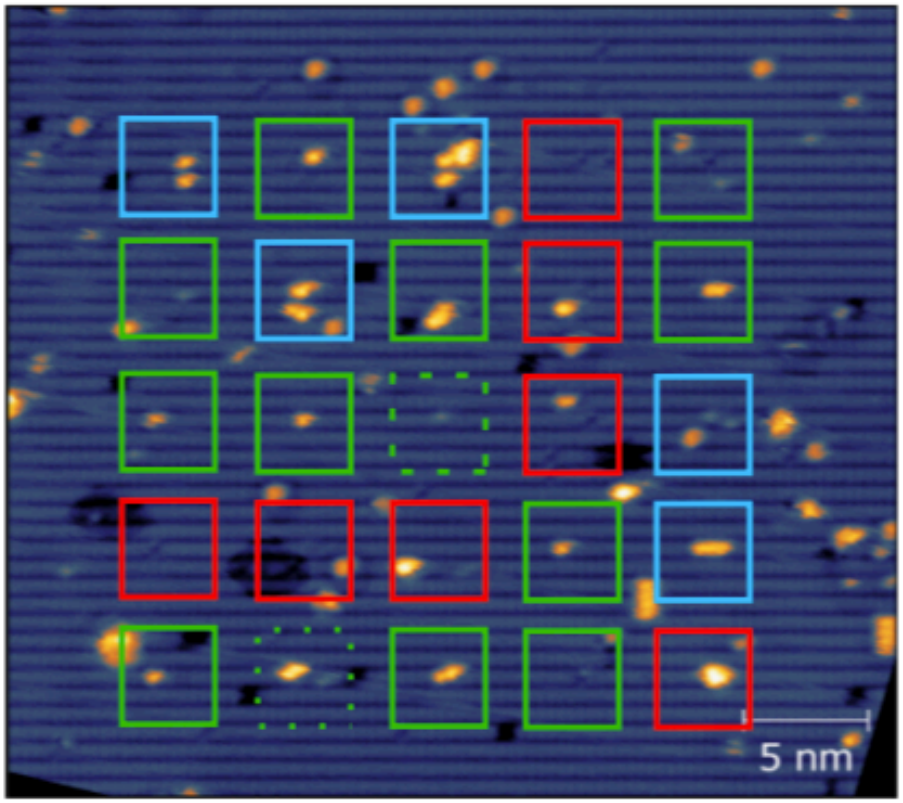


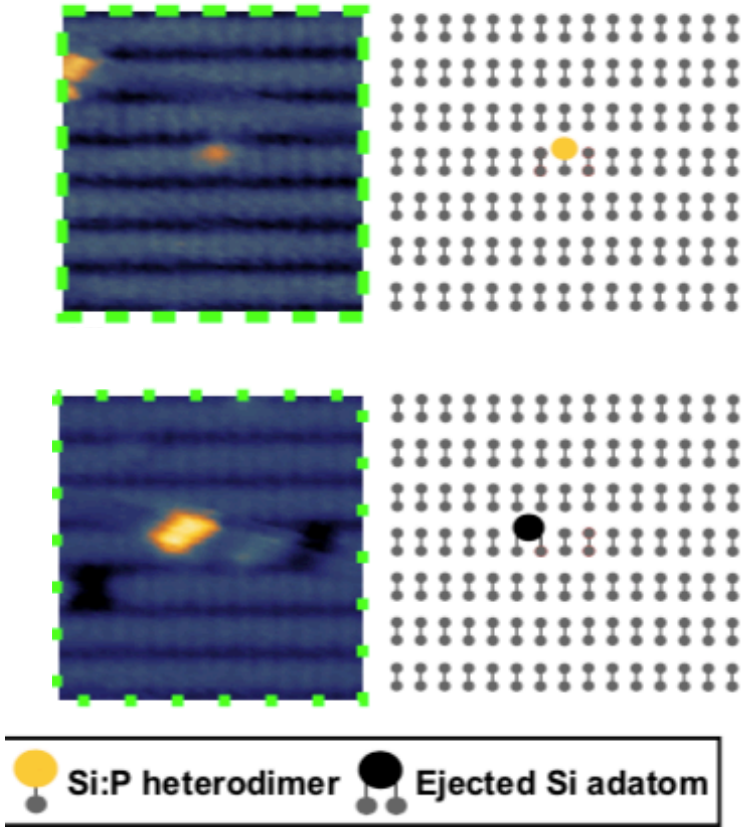


Using STM, we can make a perfect three dimer window ~58% of time
See Justin Koepke's talk for experimental details! Session L29.00009, Wednesday 10:00 am CDT

Single donor incorporation rate

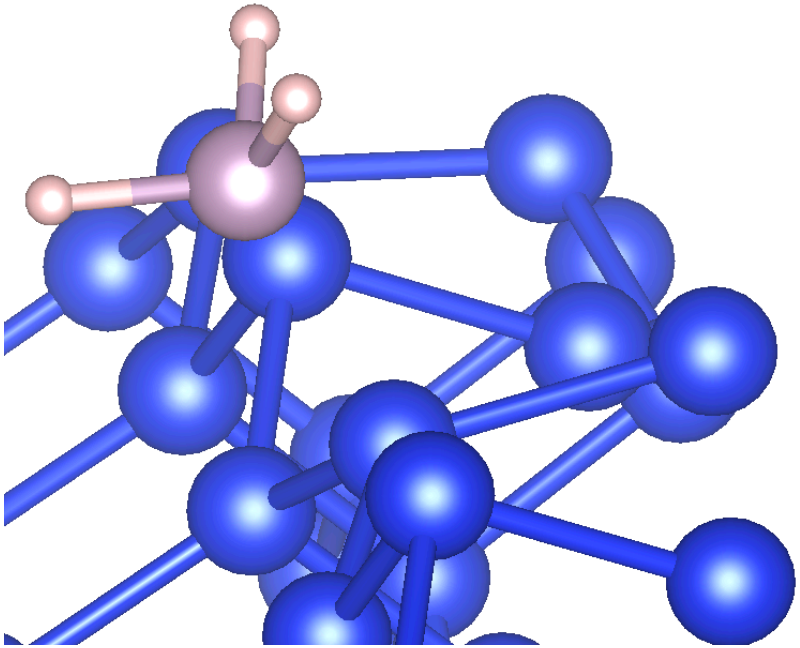
$$P(N) = \left(\sum_{w} P_L(w) P_I(n = 1|w) \right)^N$$





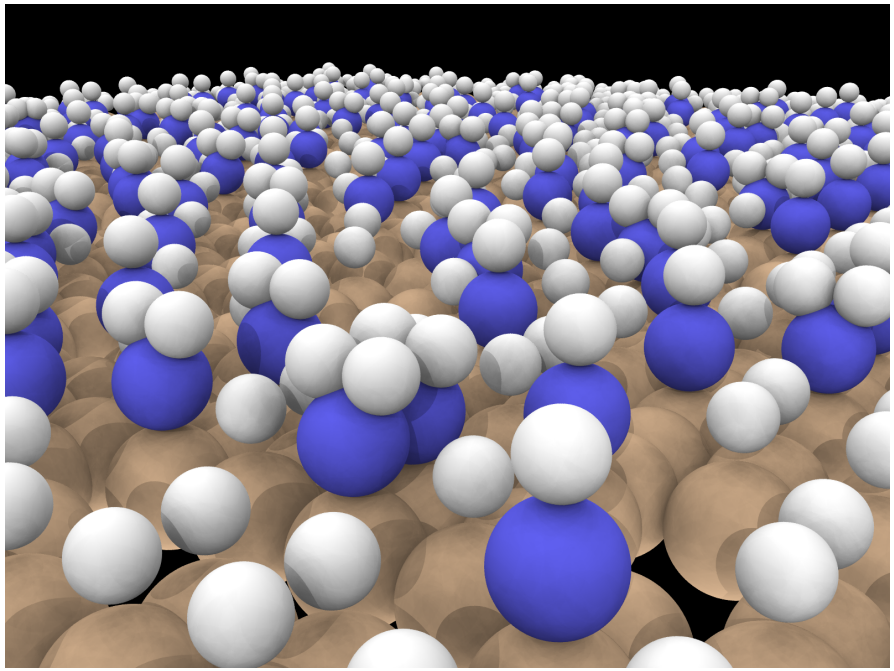
Given a perfect 3 dimer window, we find P(Incorporation) = 63% ± 10%

Creating a chemical model for incorporation



Density Functional Theory

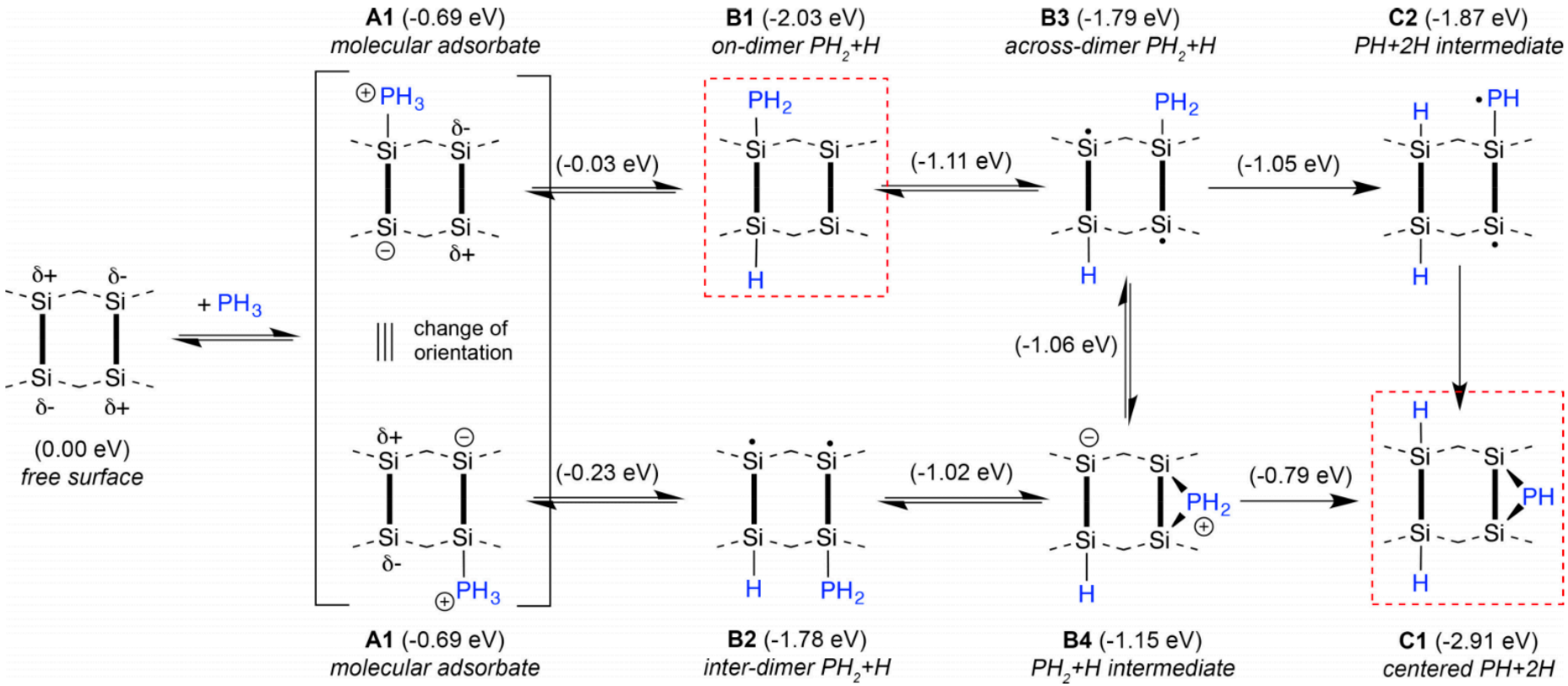
Reaction Pathways of Phosphine Gas



Kinetic Monte Carlo

Geometry and Probability of incorporation

Old reaction chemistry from Density Functional Theory

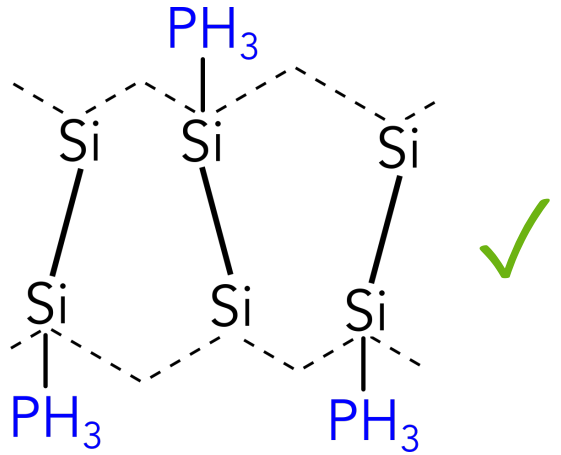


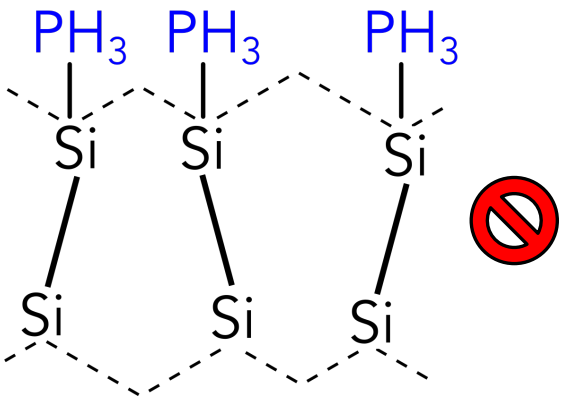
Accept a bridging PH as incorporated

Warschkow et al., *J. Chem. Phys.*, **144**, 014705 (2016).

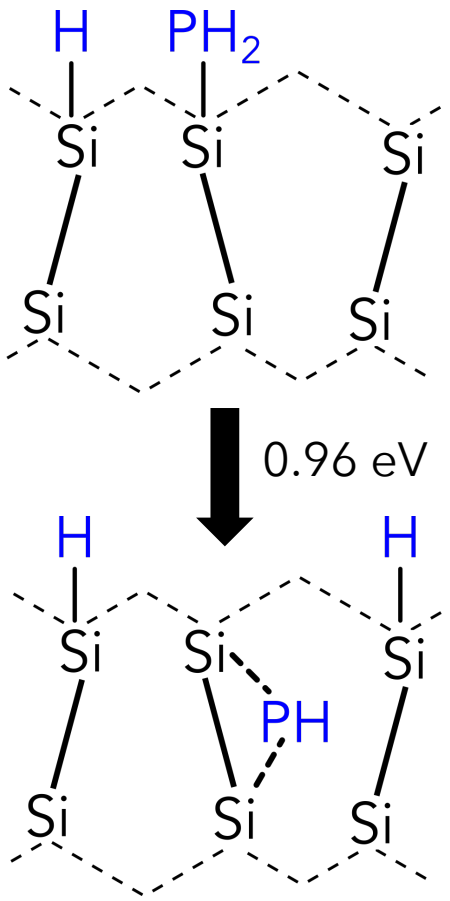
New reaction chemistry from Density Functional Theory

PH_3 adsorbs on lower sites





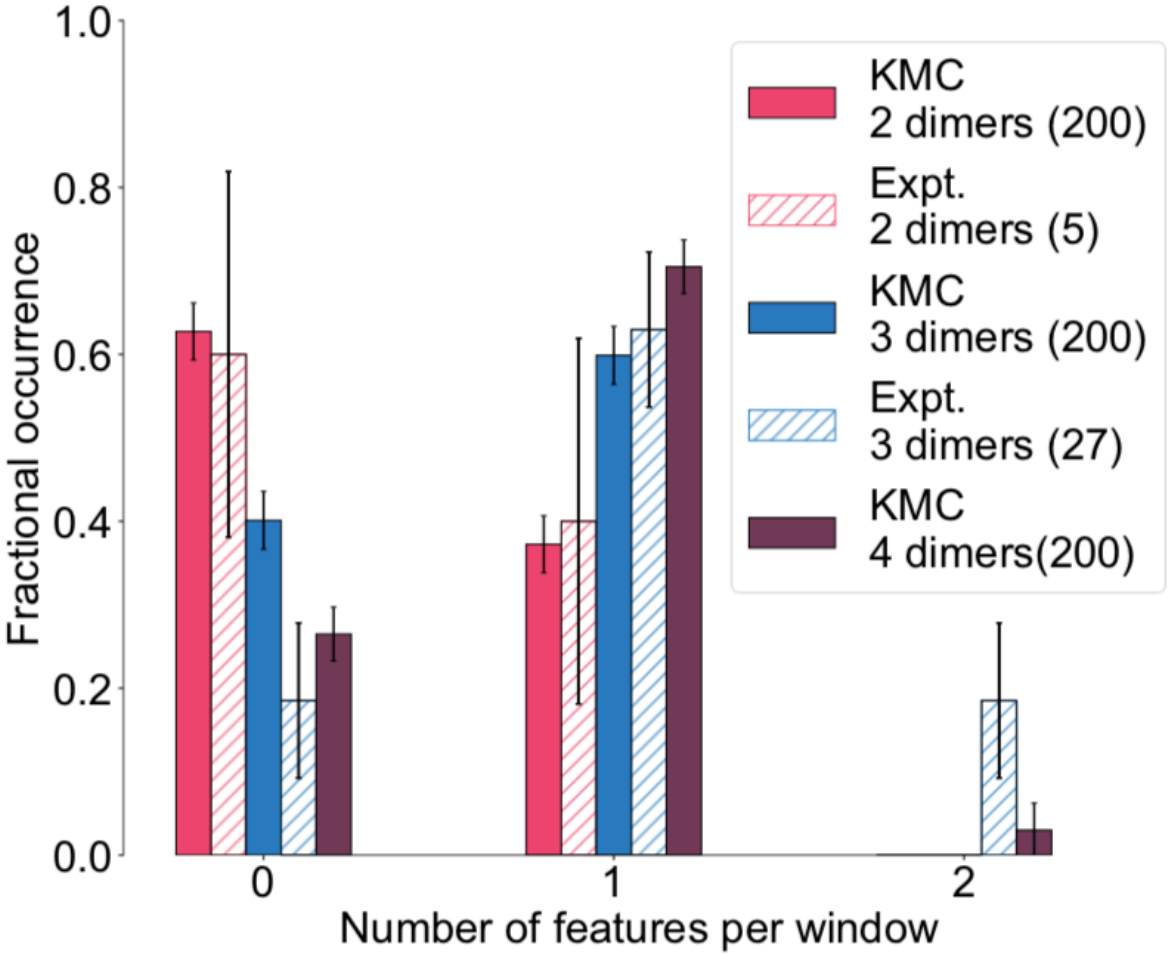
New concerted reaction



Reaction for Phosphorus incorporation is thermodynamically downhill with manageable reaction barriers

Additional calculations from Peter Schultz (Sandia)

Kinetic Monte Carlo (KMC) prediction of incorporation rates



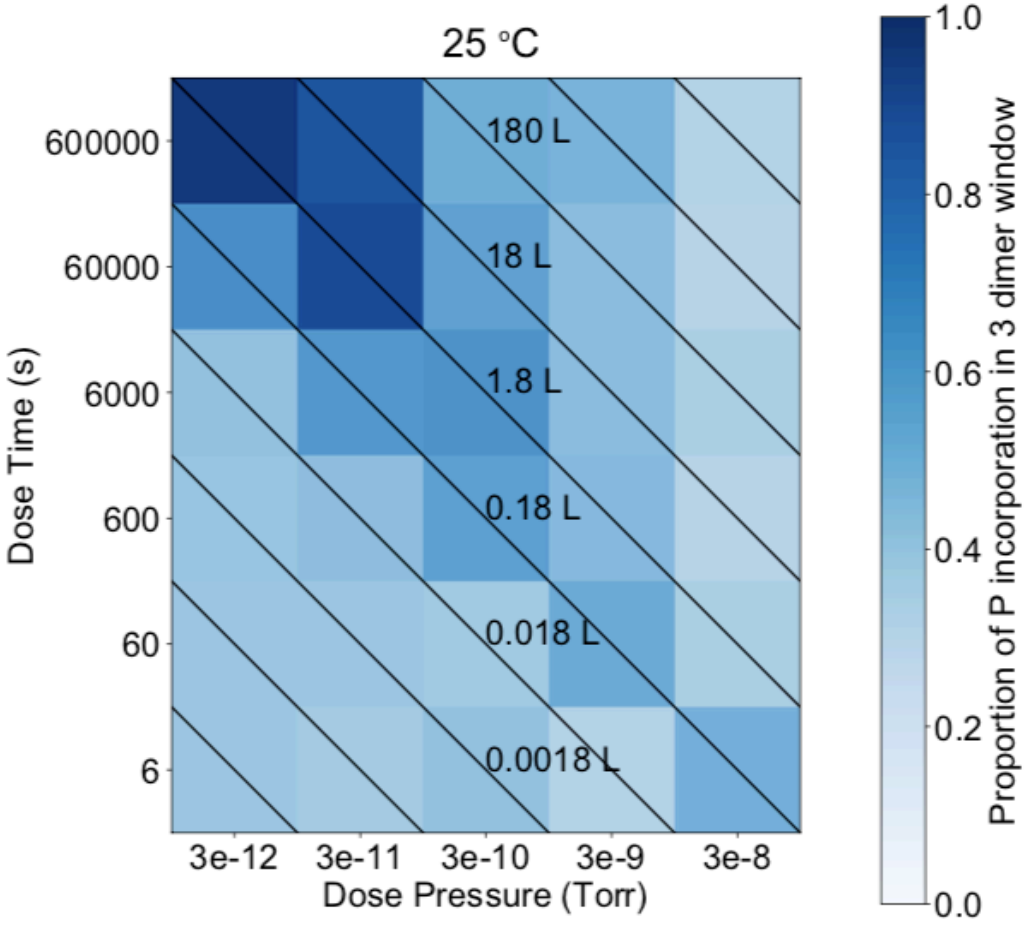
$$\Gamma = A \exp \Delta / k_{\mathrm{B}} T$$

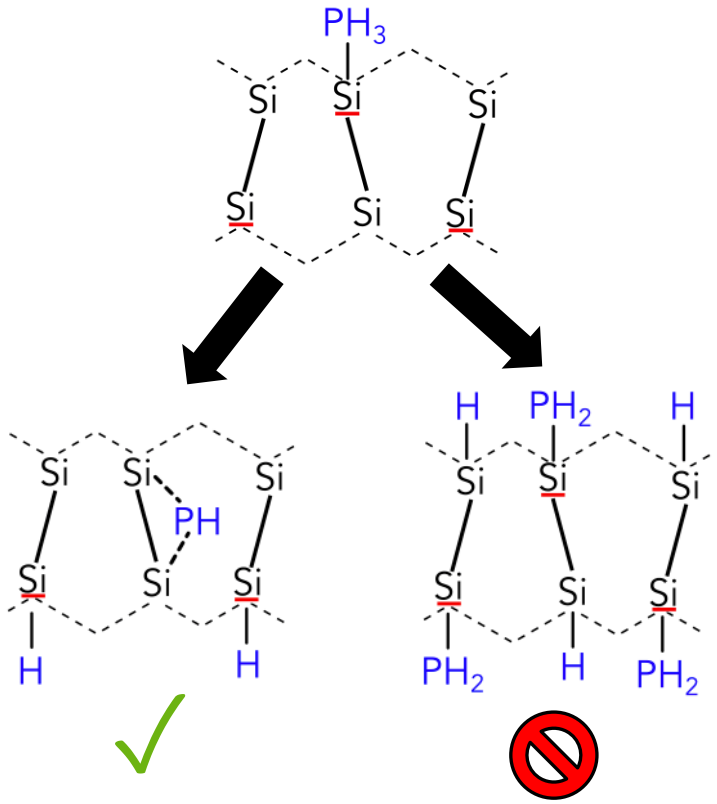
Dose phosphine at room T, 3x10^{-10} Torr, 10 minutes (0.18 L coverage)

Anneal at 310 °C for 10 seconds

KMC model matches experimental incorporation rates for 2 and 3 dimer windows within statistical uncertainty. Predicts a stochastic process.

Can we achieve deterministic incorporation?

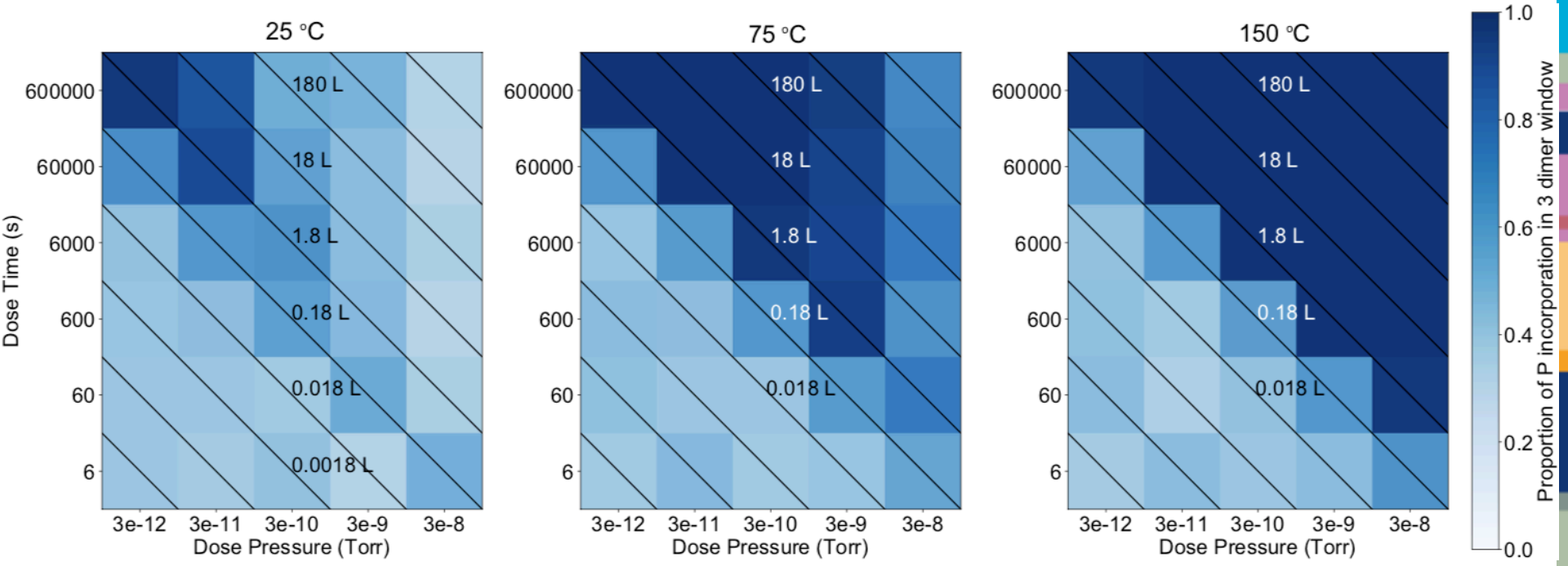




If phosphine has enough time and space to fully dissociate before another phosphine adsorbs in the same window, it *will* incorporate!

Giving phosphine enough time and space…

Dose temperature

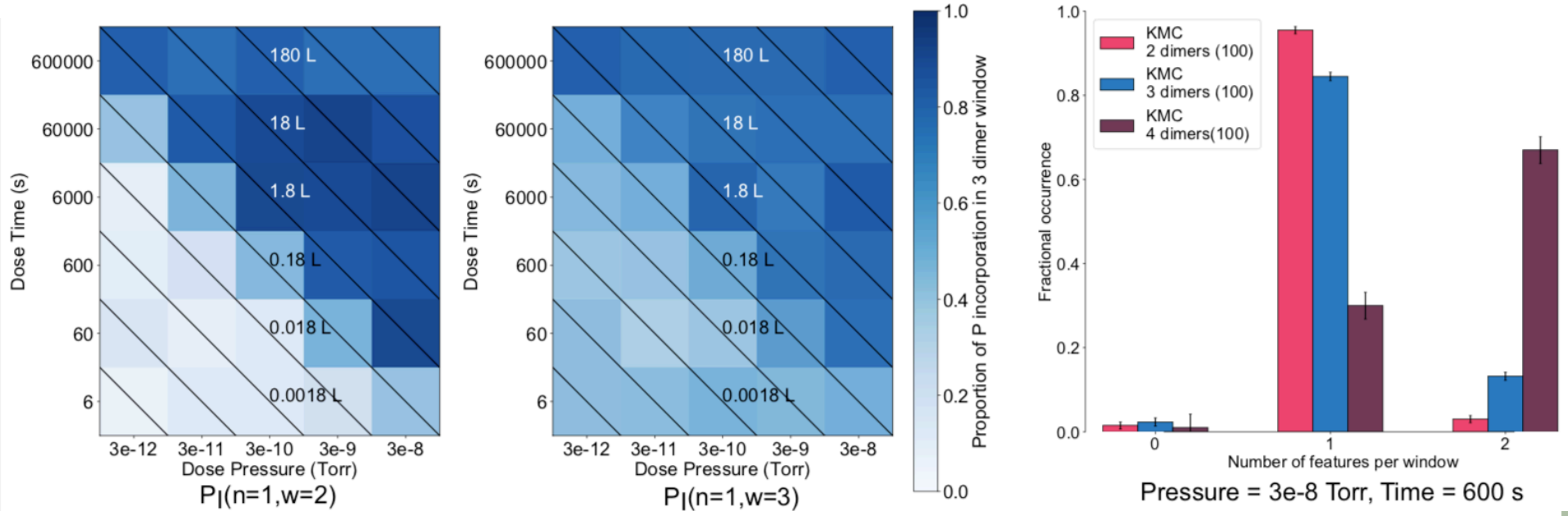


We predict that reducing pressure while increasing dose time, or increasing dose temperature leads toward deterministic incorporation

Deterministic incorporation at comparable pressures, low temperatures

Dose phosphine at 100 K

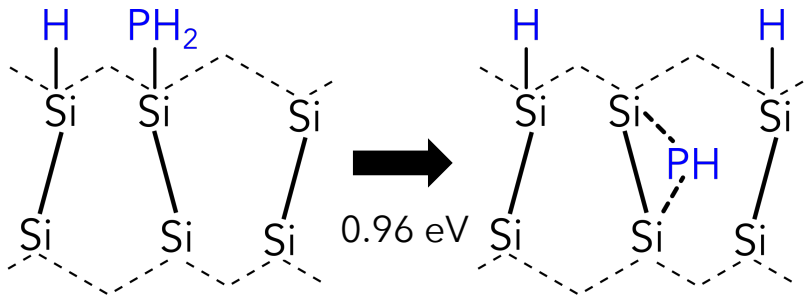
Anneal at 400 °C for 10 seconds

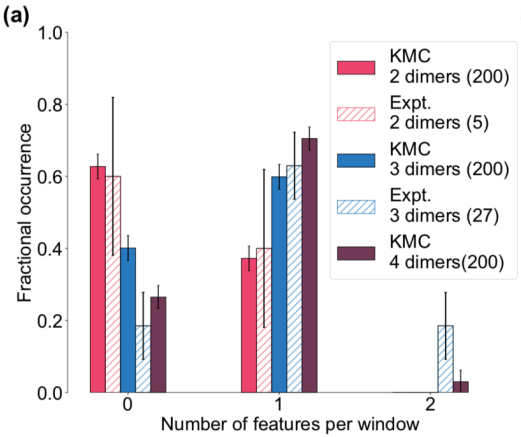


Alternatively we can imagine dosing at very low temperatures to suppress dissociation, saturating the window. Then when you anneal, most phosphine quickly desorb, leaving one to fully dissociate; essentially deterministic

Method developed in: Simmons and Keizer, Patent, WO2019/210370A1 (2019).

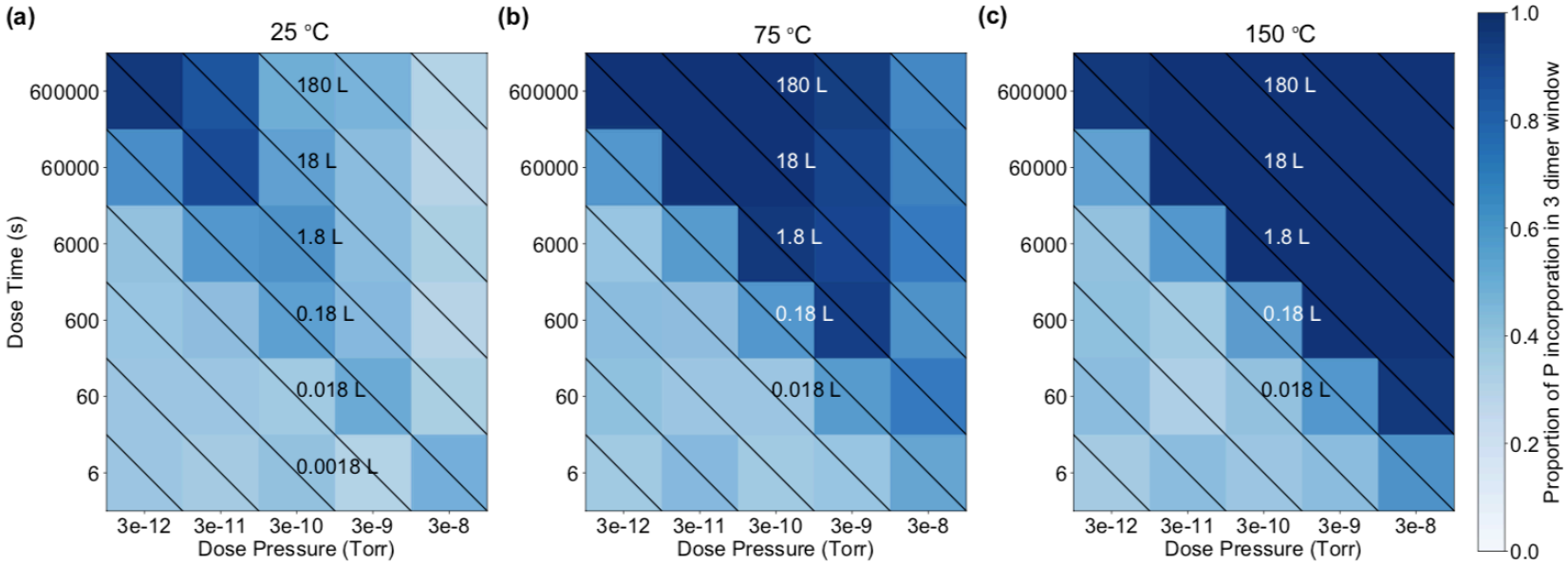
Summary





Density Functional Theory

Kinetic Monte Carlo



For thoughts on what missing a donor would do to transport measurements, see Mitchell Brickson's talk! Session E29.00011, Tuesday 10:24 am CDT

Collaborators

Theory:

Mitchell Brickson
Andrew Baczewski
Peter A. Schultz
Richard Muller

Experiment:

Jeffrey Ivie
Justin Koepke
Andrew Mounce
Ezra Bussmann
Shashank Misra

Full paper coming to an arxiv near you soon!
KMC code will be posted at: https://github.com/quantumquinn/apam-kmc

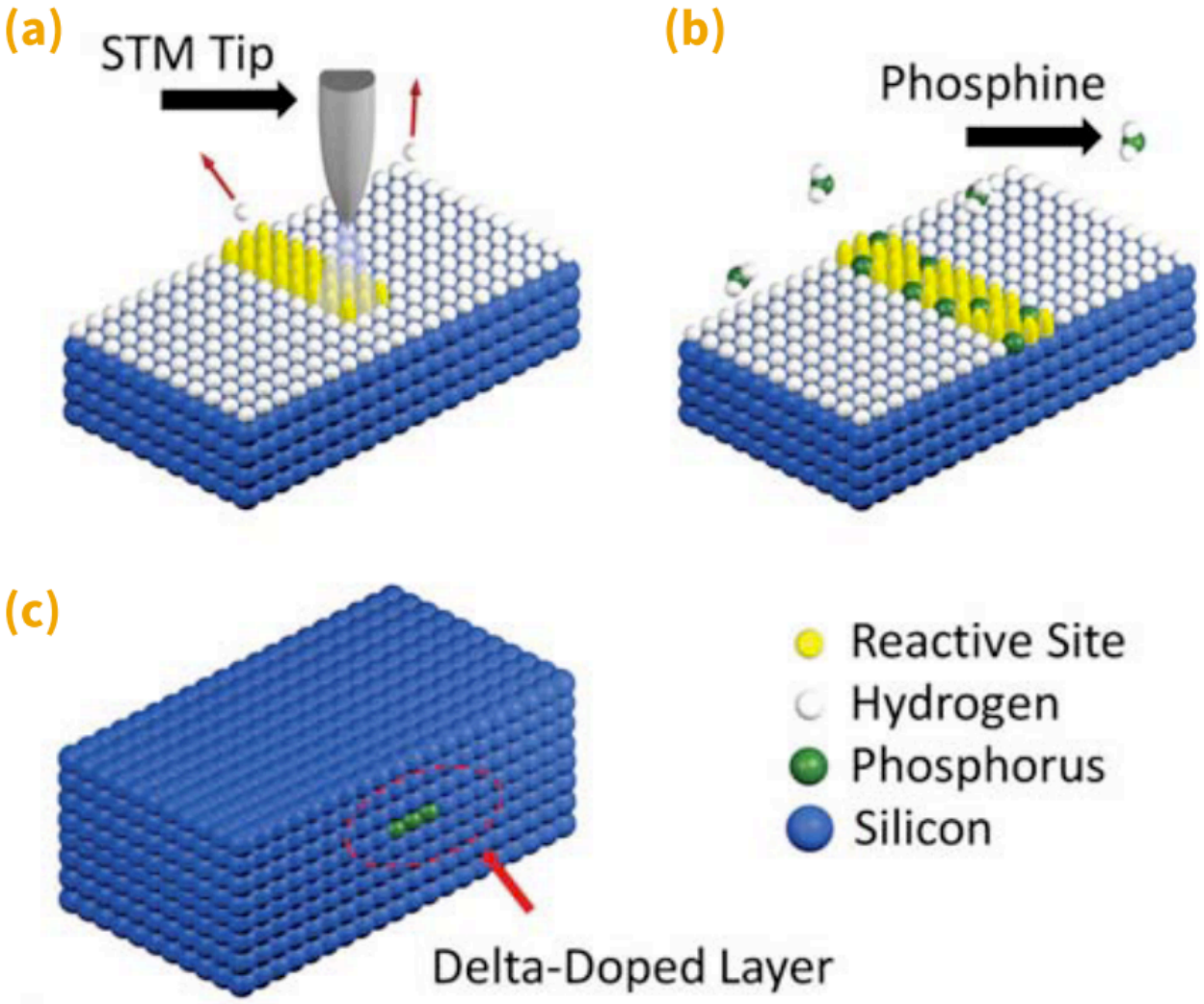
Thanks for your attention!

Sandia National Laboratories

This work was supported by the Laboratory Directed Research and Development Program at Sandia National Labs. Sandia National Laboratories is a multi-missions laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for DOE's National Nuclear Security Administration under contract DE-NA0003525.

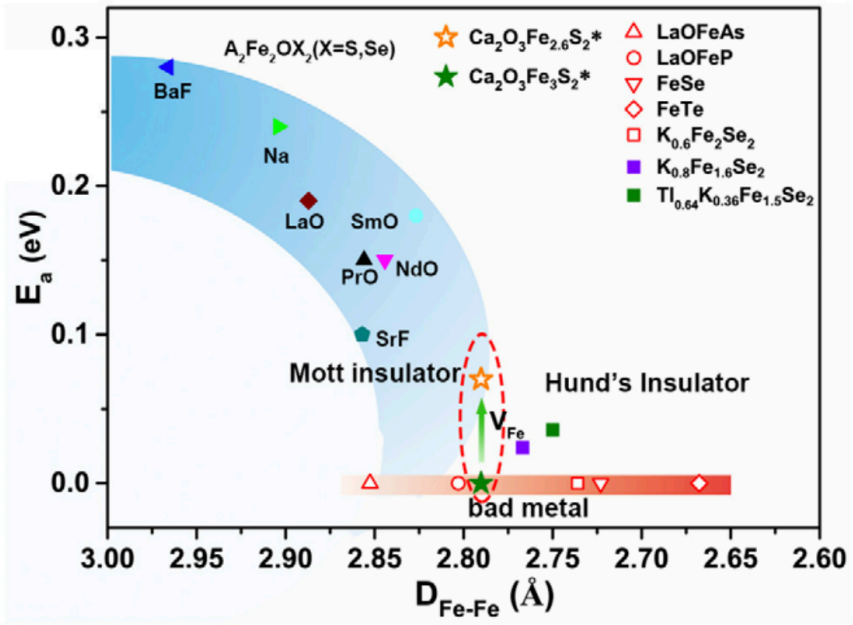
CCR Center for Computing Research

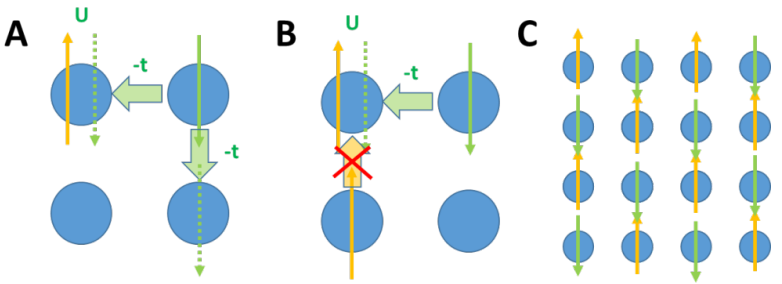
Atomic Precision Advanced Manufacturing (APAM)

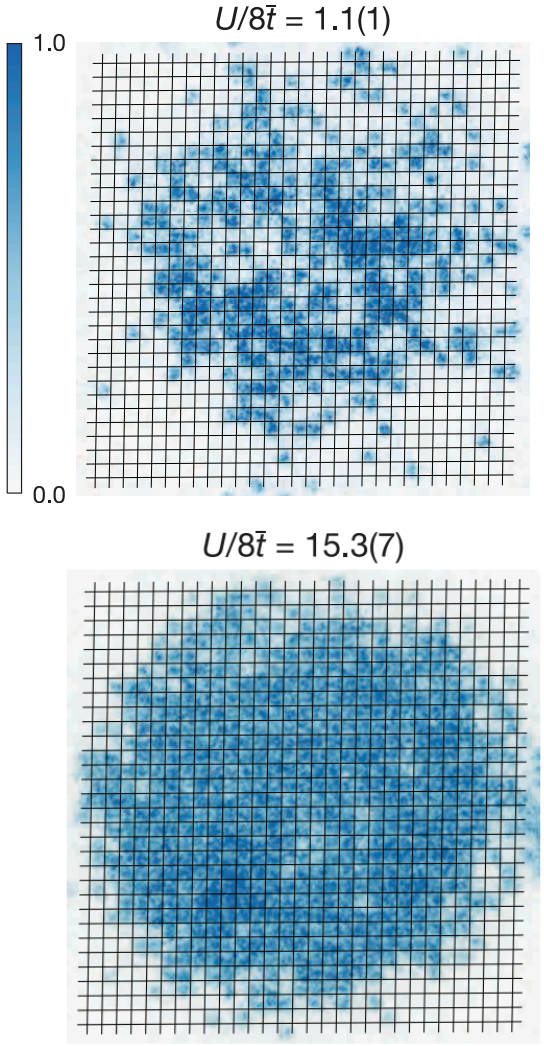


Ward et al., *Electronic Device Failure Analysis*, **22**, 1 (2020).

Designer Quantum Materials







Analog simulations of difficult to solve quantum systems such as Fermi-Hubbard model

Zhang et al., *J. Phys. Cond. Mat.*, **28**, 145701 (2016).

Greif, et al., *Science*, **351,** 6276, 953-957 (2016)