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Pathways for atomic-precision incorporation of donors and acceptors in silicon

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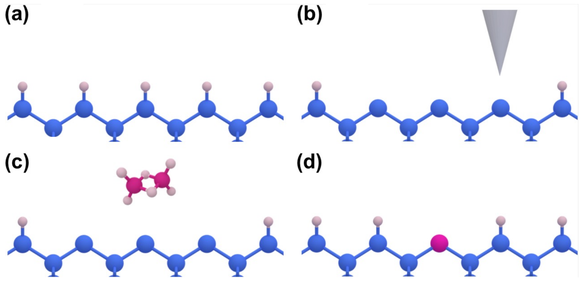
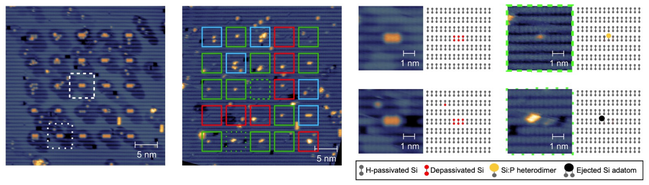
Atomic-Precision Doping of Silicon via STM Hydrogen Lithography

Atomic-precision methodology using STM lithography [1]



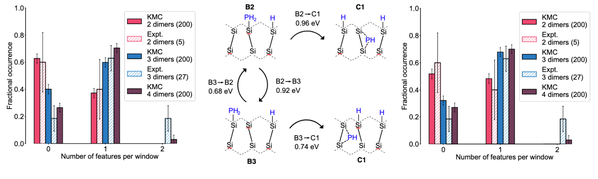
STM lithography creating and measuring single donor windows [2]



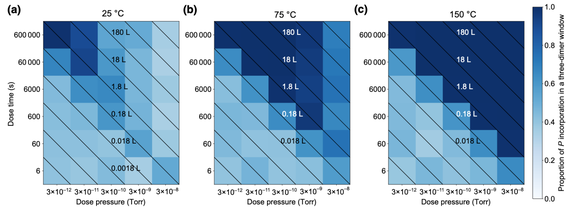
- Use Scanning Tunneling Microscopy (STM) lithography and then subsequent chemical precursor exposure for atomic-precision doping of Si(100)-2x1 surface
- We develop Kinetic Monte Carlo (KMC) models of incorporation for dopant precursors, using Density Functional Theory (DFT) dissociation pathways
- This allows us to predict how stochastic chemical dissociation pathways and dosing conditions affect dopant incorporation
- We examine pathways of PH_3, B_2H_6, BCl_3, $AlCl_3$

Single Donor Doping

Probability of donor incorporation as a function of depassivated window width [2]



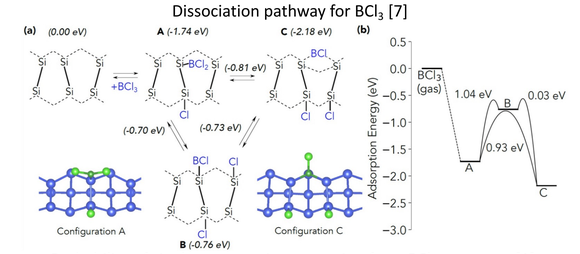
Dosing conditions and temperature can drastically affect incorporation rates [2]



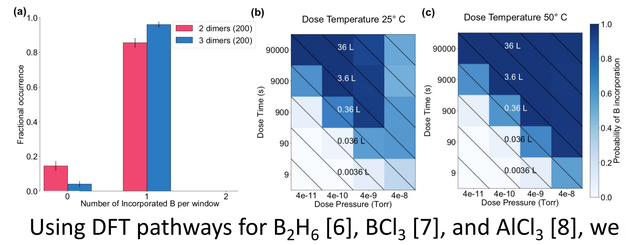
- Stochastic phosphine dissociation leads to sub-deterministic incorporation of a single donor in a three dimer wide window (see also [3,4,5])
- We predict incorporation rates matching experiments at room temperature and that **higher temperatures can lead to deterministic incorporation of a single donor, which is needed for reliable qubit arrays!**

Single Acceptor Doping

Dissociation pathway for BCl_3 [7]



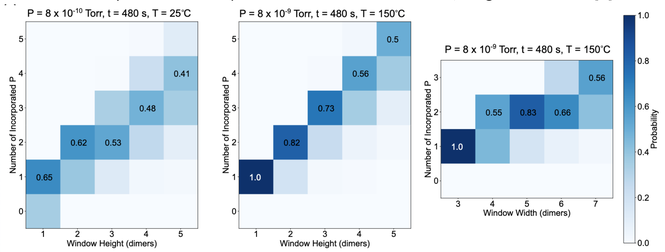
Probability of single acceptor incorporation from BCl_3 precursor [1]



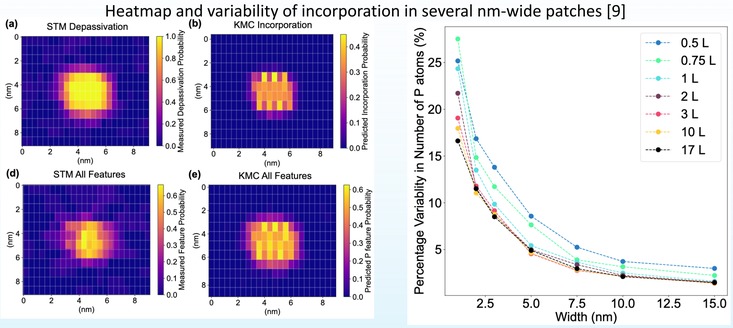
- Using DFT pathways for B_2H_6 [6], BCl_3 [7], and $AlCl_3$ [8], we predict single acceptor incorporation rates in three dimer wide windows
- We predict BCl_3 and $AlCl_3$ are likely candidates for **deterministic single hole incorporation** due to simple dissociation pathway
- May enable reliable acceptor spin-based qubit arrays!

Multi-donor Doping

Probability of donor incorporation as a function of width, height of window [9]



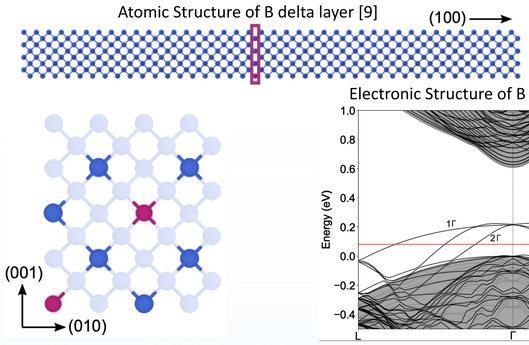
Heatmap and variability of incorporation in several nm-wide patches [9]



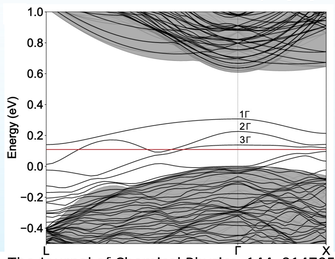
- Analog Quantum Simulations require variation in number of donors in patches to be small in order to have a well defined Hamiltonian [10]
- We predict that creating slightly larger depassivation windows, even 2x3 dimers wide, **can give a probability > 99% of at least one donor incorporating at room T**
- We examine typical lithographic and chemical variation in the creation of 3 nm x 3 nm wide patches, showing that the incorporation rate is highly robust to both types of errors
- We predict that variation in the number of incorporations is largely a function of edges, and % variation decreases as the patch size increases

Acceptor Delta Layer Electronic Structure

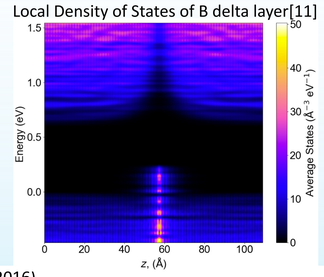
Atomic Structure of B delta layer [9]



Electronic Structure of Al delta layer [11]

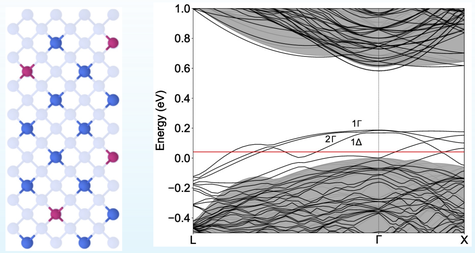


Local Density of States of B delta layer [11]



- We use DFT to examine the electronic structure for acceptor delta layers, examining ¼ monolayer coverage
- We predict that both the type of acceptor (B vs Al) and the placement of dopants (ordered vs disordered) can be used to tune the band structure and effective mass of acceptor induced valence bands

Atomic and Electronic Structure of disordered B delta layer [11]



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References: [1] Campbell, Q. et al., AVS Quantum Science 4 (1), 016801 (2022).
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[4] Füchsle, M., PhD Thesis, UNSW (2011).
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[6] Campbell, Q. et al., The Journal of Physical Chemistry C 125 (1), 481 (2021).
[7] Campbell, Q. et al., arXiv:2201.11682 (2022).
[8] Radue, M. S. et al., The Journal of Physical Chemistry C 125 (21), 11336 (2021).
[9] Campbell Q. et al., arXiv:2207.10631 (2022).
[10] Kiczynksi, M. et al., Nature 606, 694 (2022).
[11] Campbell Q. et al., In Preparation (2022).

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