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Sandia National Laboratories

A multiscale model of the reaction pathway for p-type doping using diborane on Si(100)-2x1

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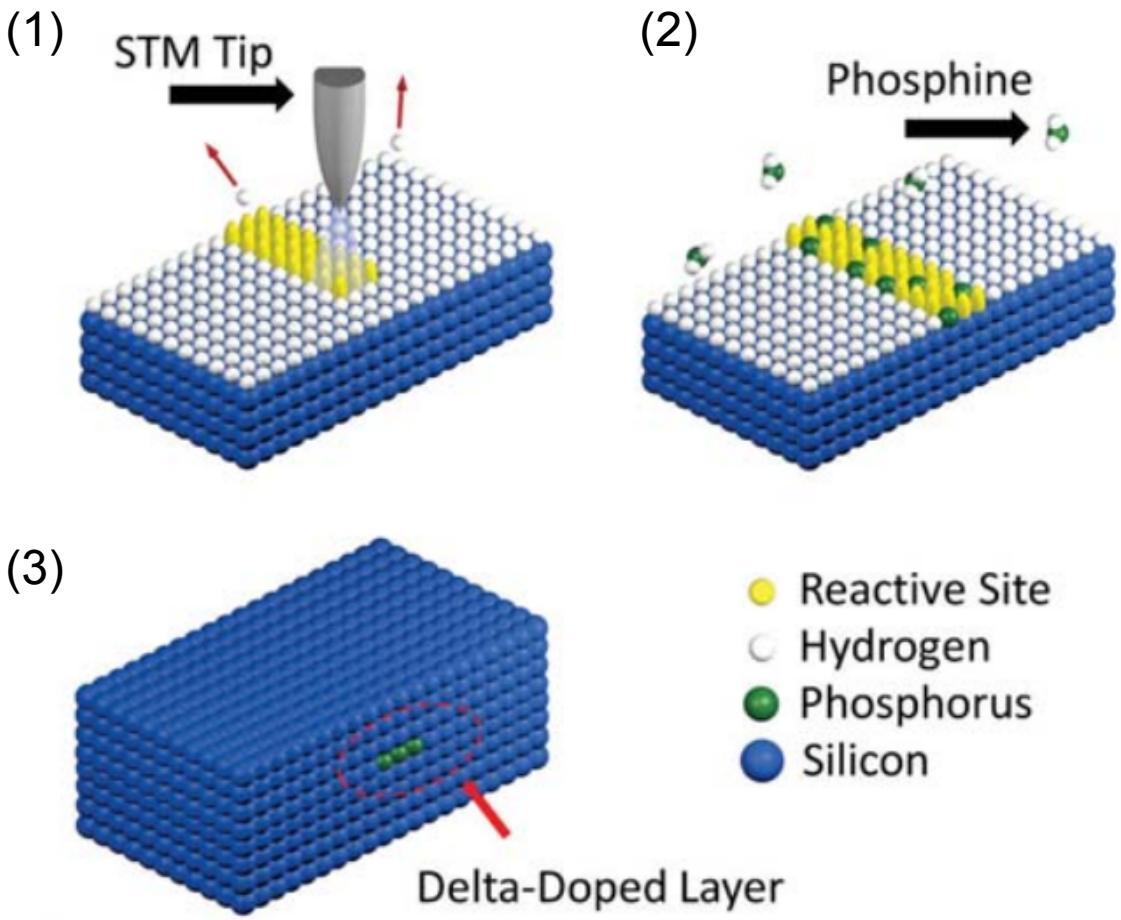
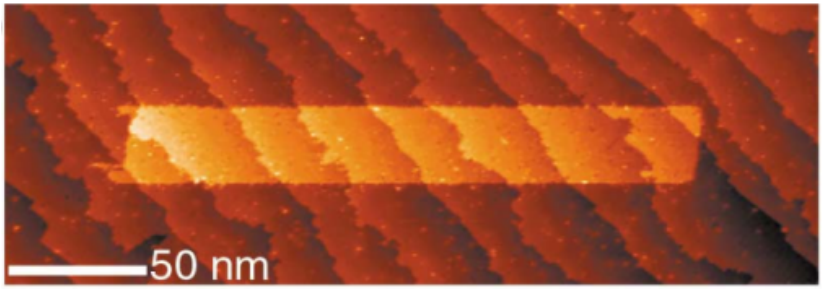
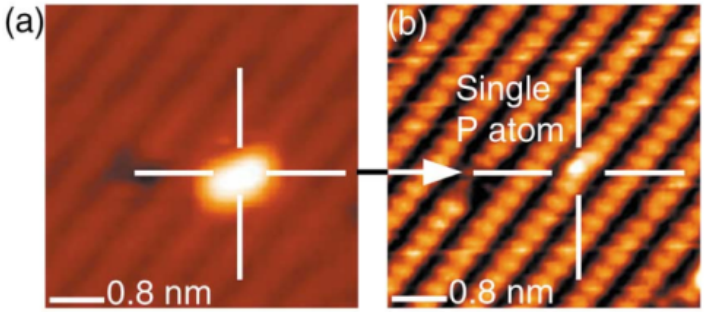
Atomic-precision doping of silicon

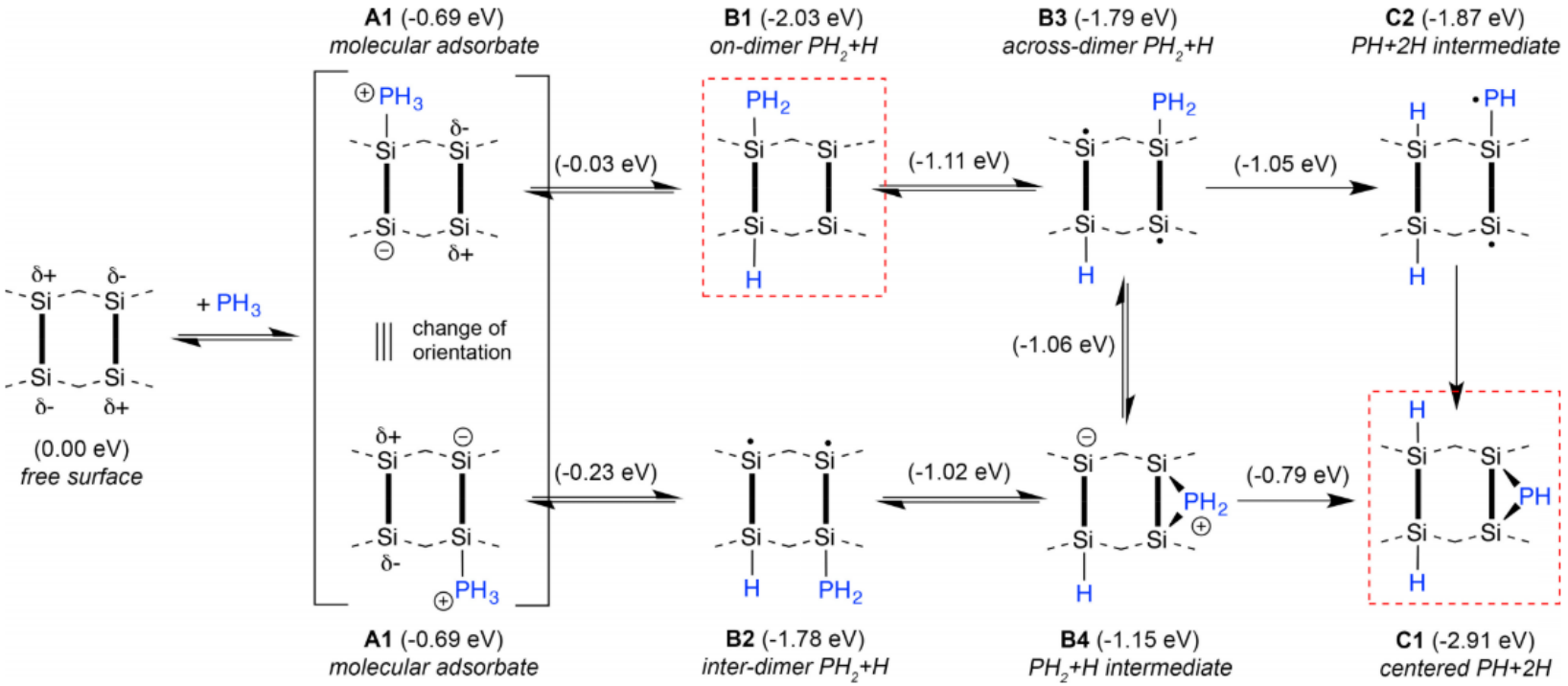


Ward *et al., Electronic Device Failure Analysis*, 22, 4-11 (2020).

Donor doping with phosphine (PH_3) precursor has been well established



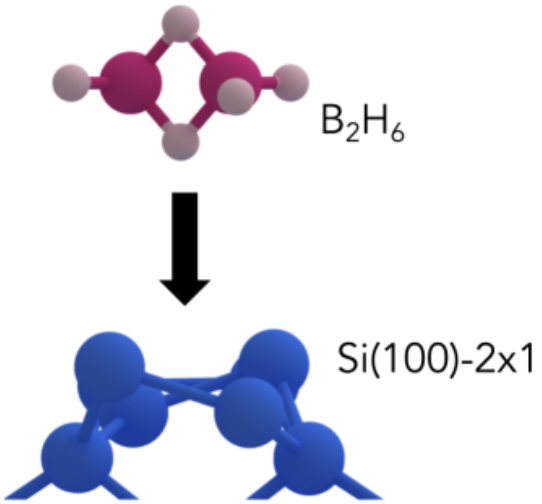


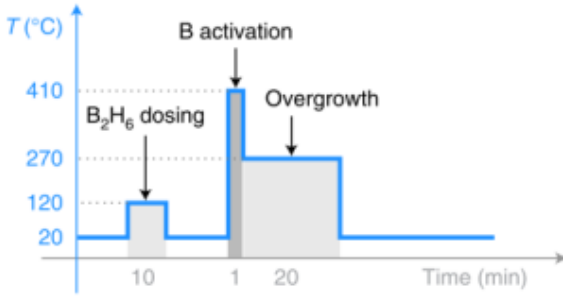


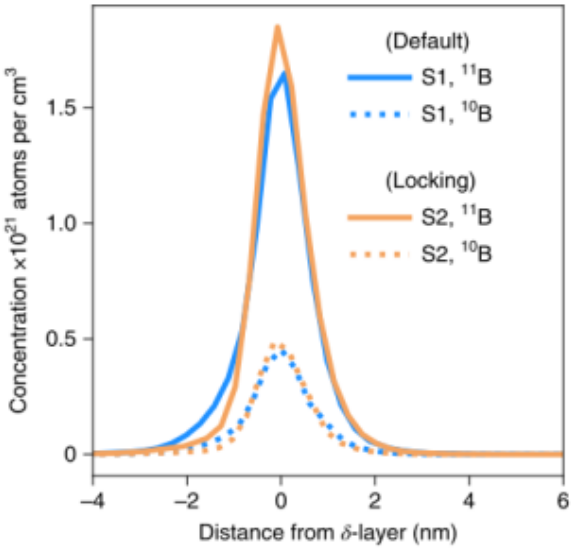
Schofield, *et al., Physical Review Letters*, 91, 136104 (2003).
Warschkow, *et al., Journal of Chemical Physics*, 144, 014705 (2016).

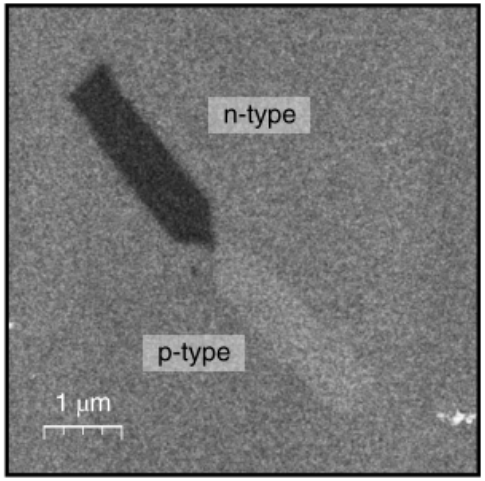
Diborane (B_2H_6) as an acceptor precursor

Škereň *et al.* recently demonstrated, high temperatures required!







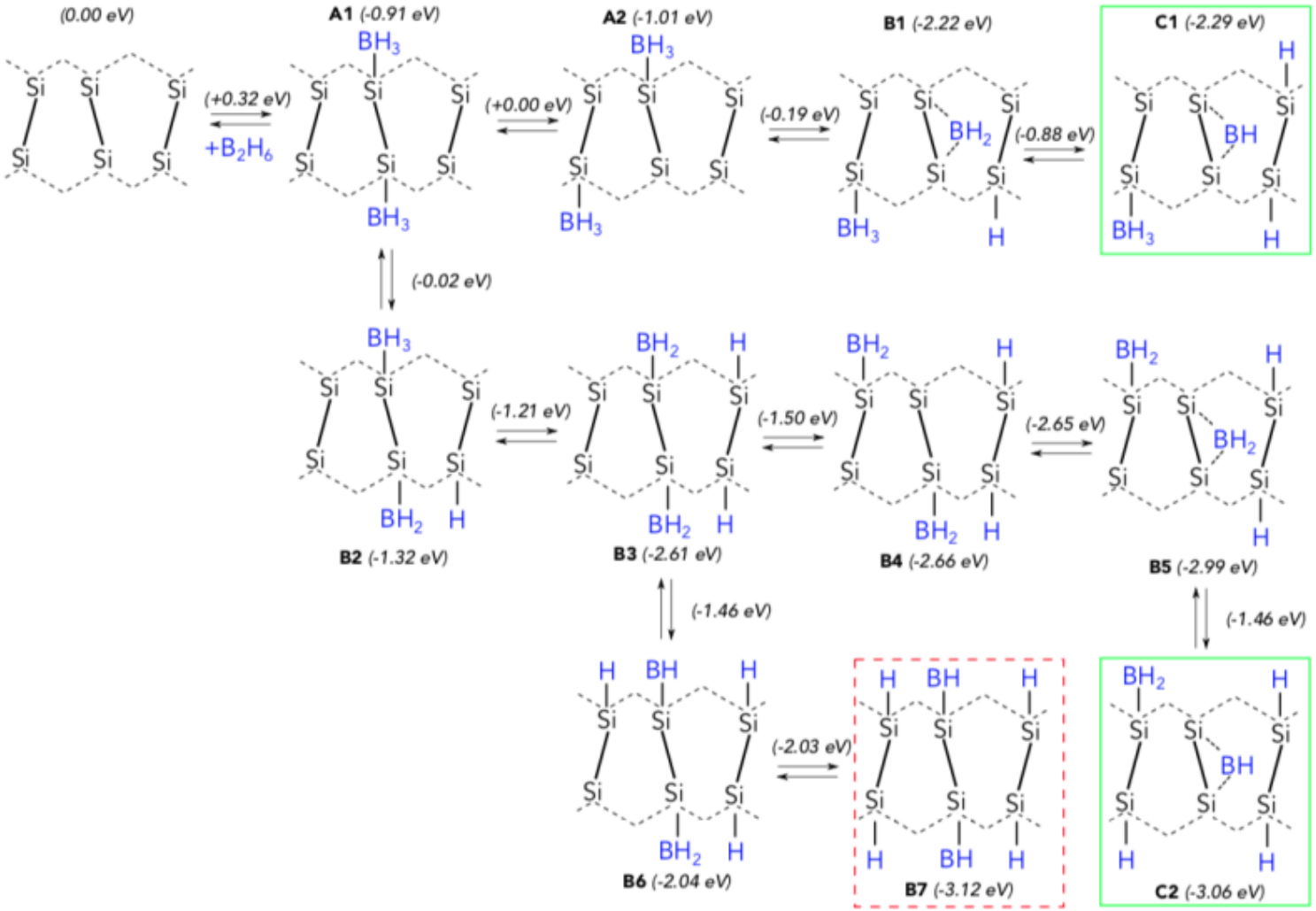


Need a theoretical model to understand and improve process

Škereň *et al.*, *Nature Electronics*, 3, 524–530 (2020).

Theoretical pathway for dissociation

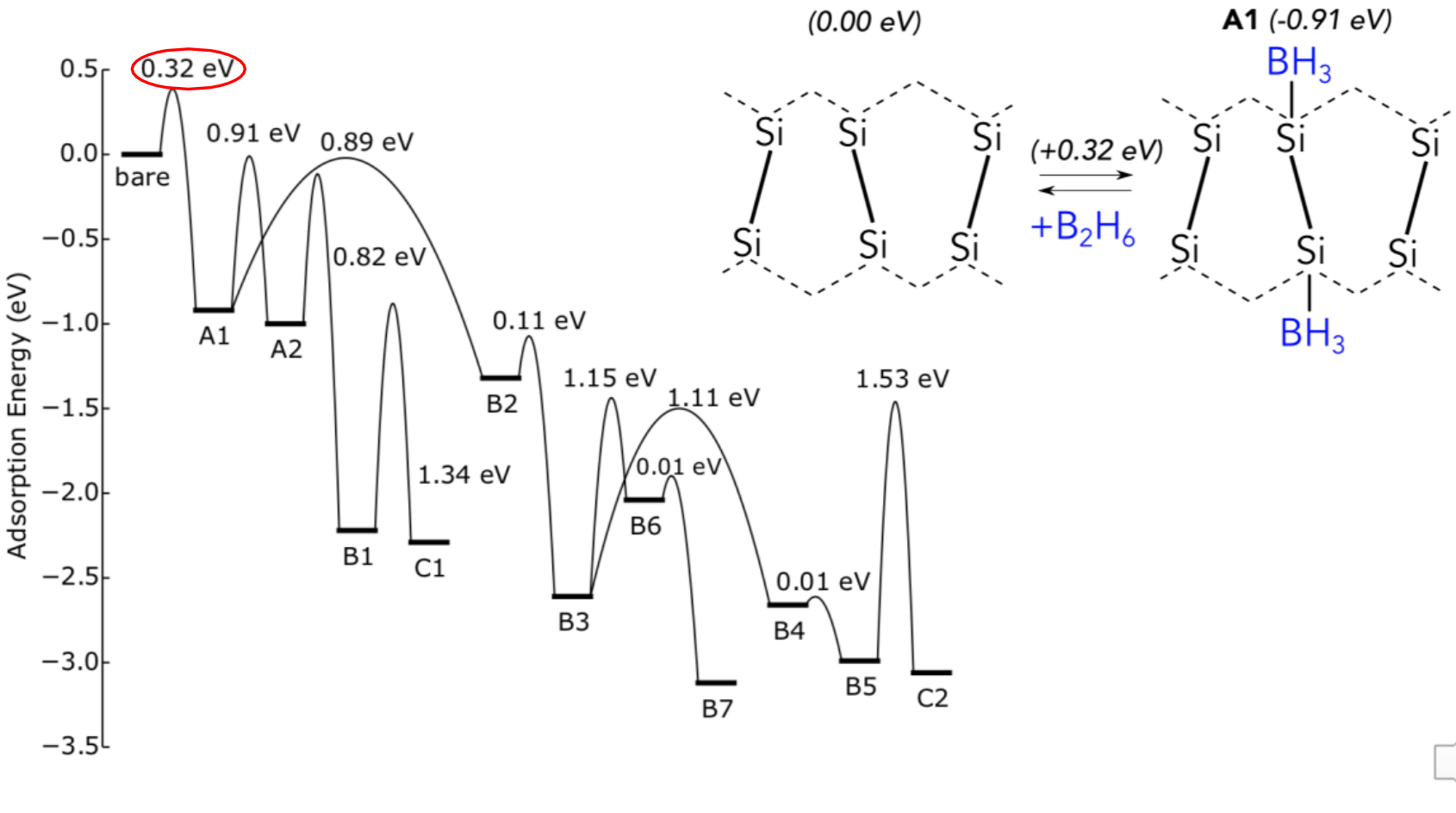
Used Density Functional Theory (DFT) to find most favorable configurations



Assuming that a bridging BH will incorporate, but BH on the same dimer row will lead to dimerized boron which will be electrically inactive

Energetic pathway

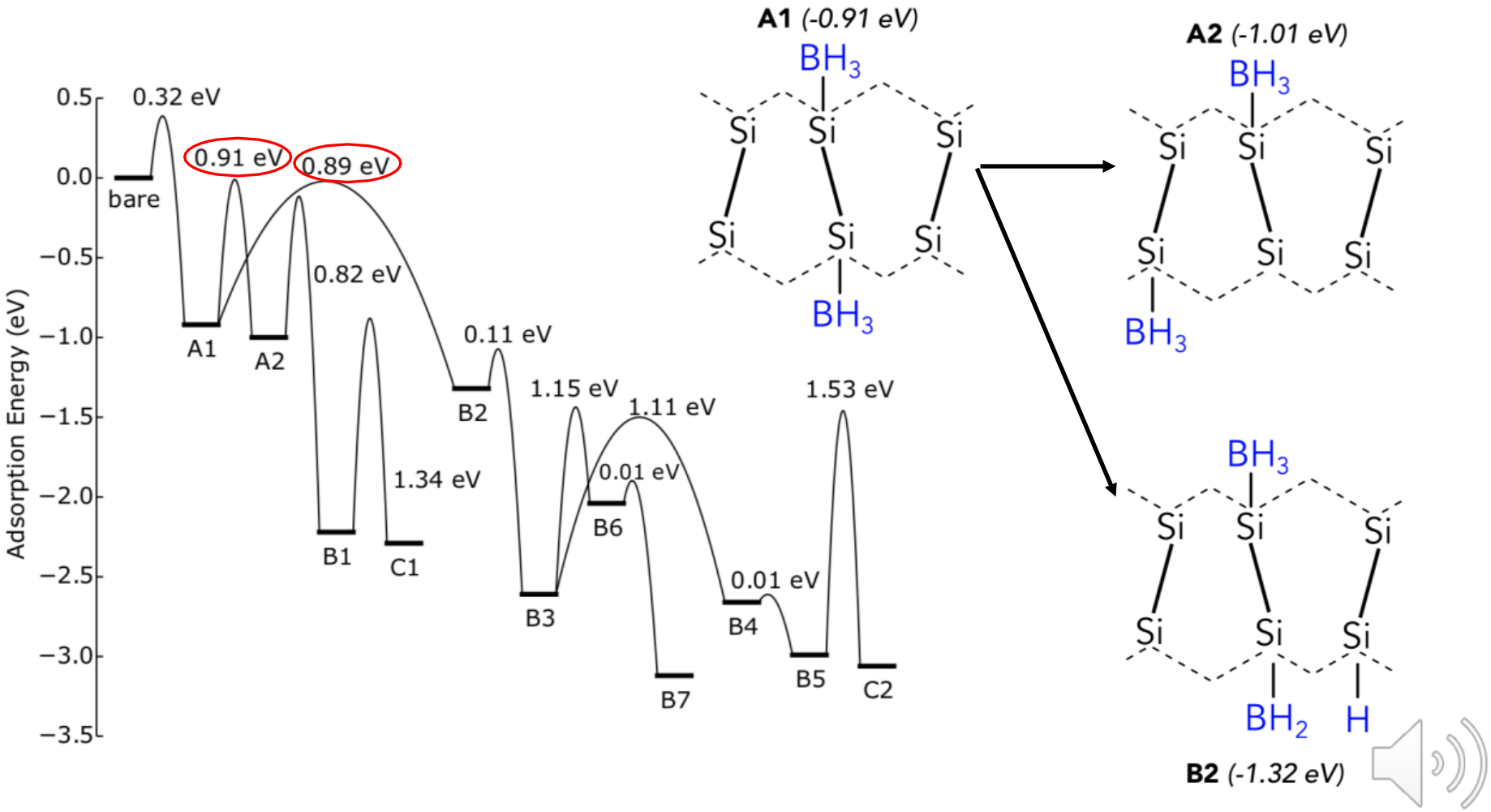
Barriers calculated using Nudged Elastic Band (NEB)



Barrier required for initial adsorption! Explains the need to heat surface during dosing

Energetic pathway

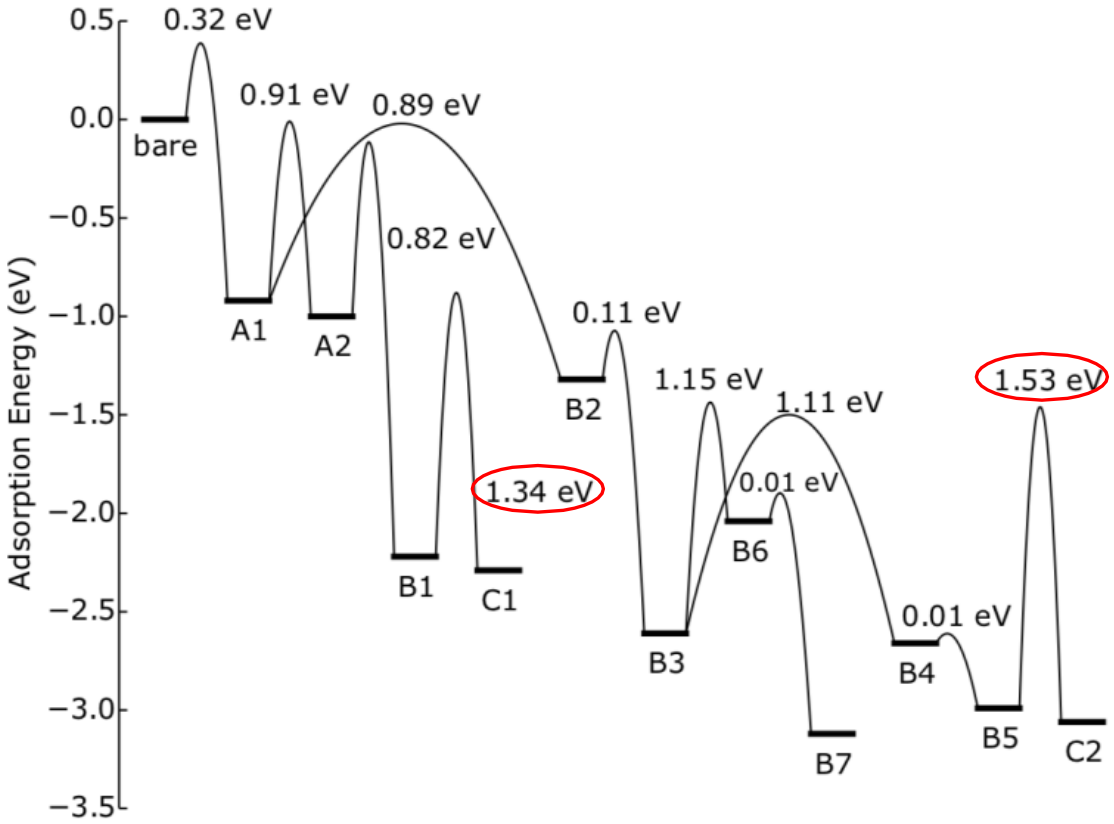
Barriers calculated using Nudged Elastic Band (NEB)



Barrier for splitting and losing hydrogen is about the same, roughly half chance

Energetic pathway

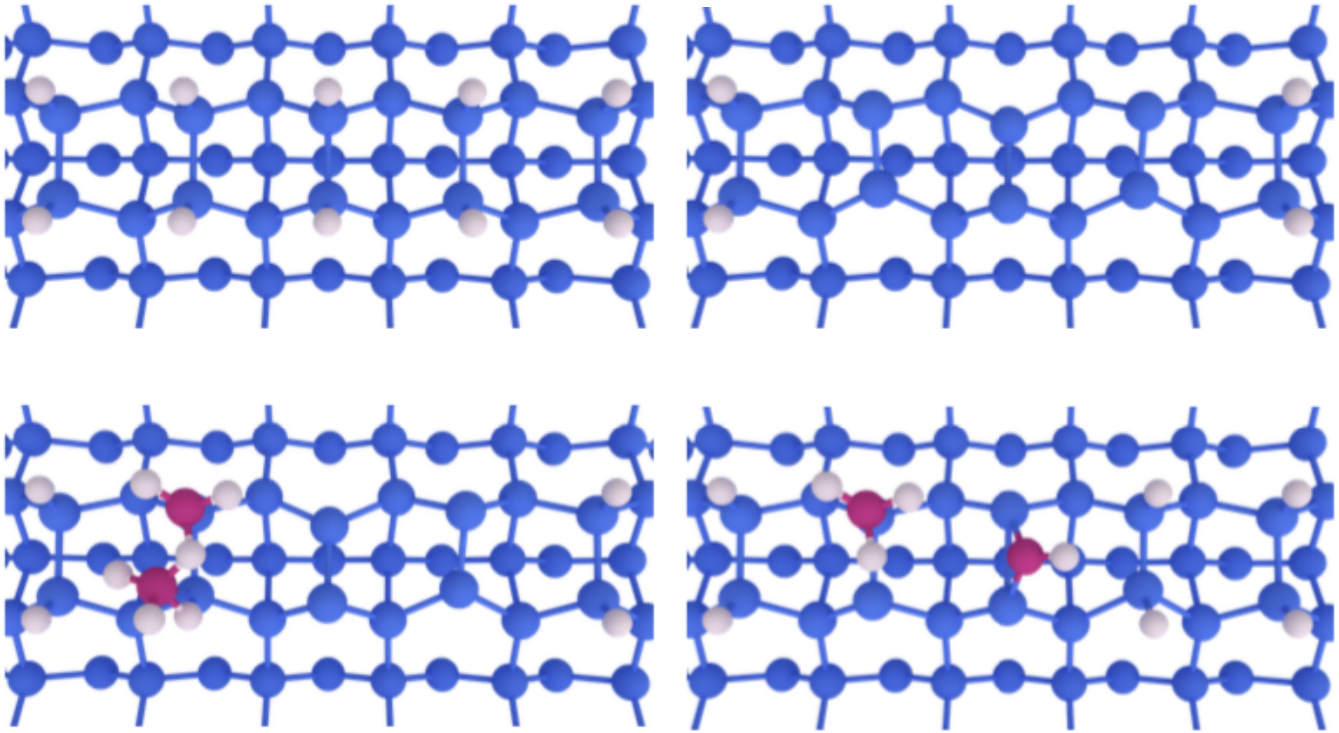
Barriers calculated using Nudged Elastic Band (NEB)



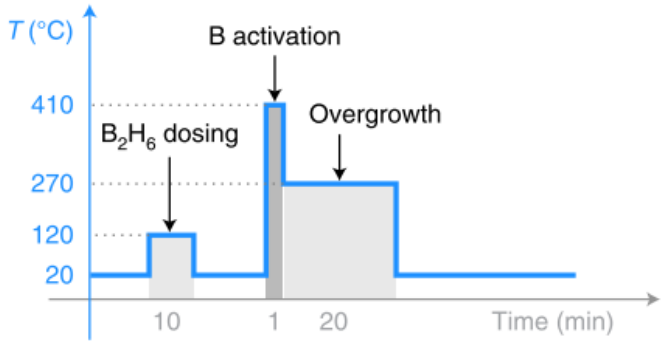
Getting to likely incorporation requires overcoming high (> 1.3 eV) barriers, which means high anneal temperatures are going to be needed

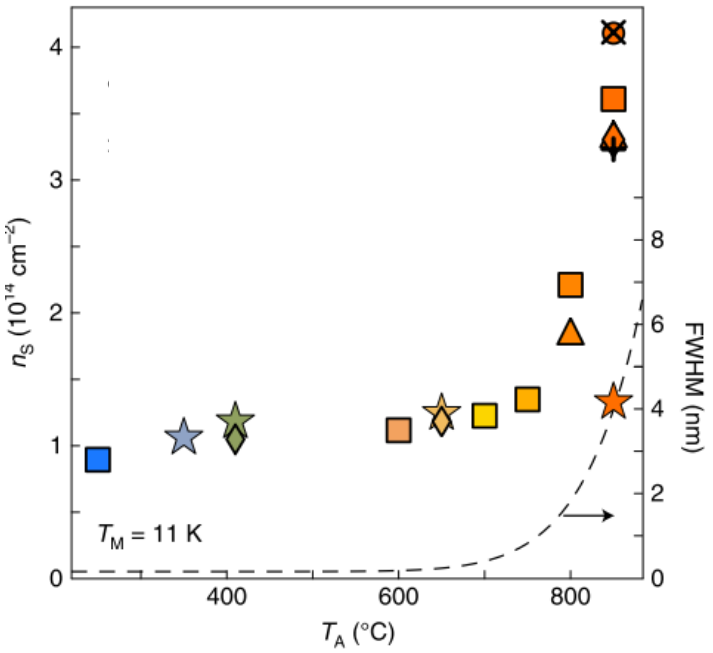
Calculate incorporation rates

Fed the calculated barriers into a Kinetic Monte Carlo (KMC) model to calculate rates and probability of incorporation

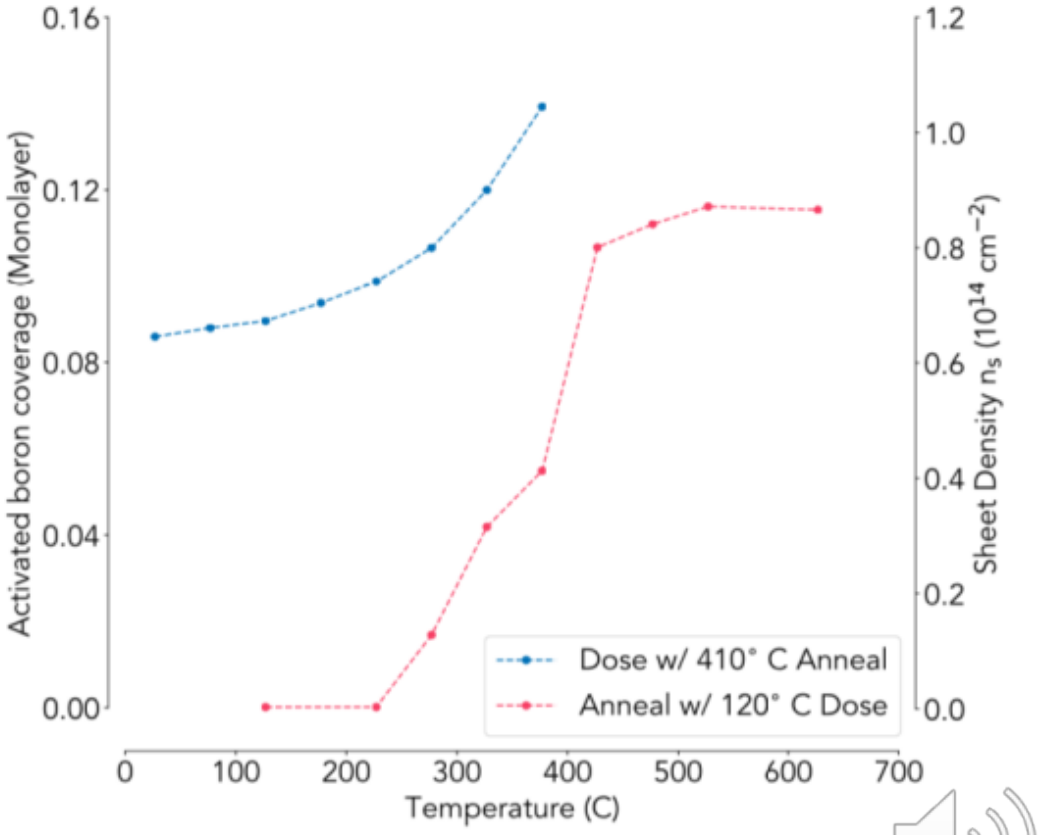


Incorporation as a function of processing parameters





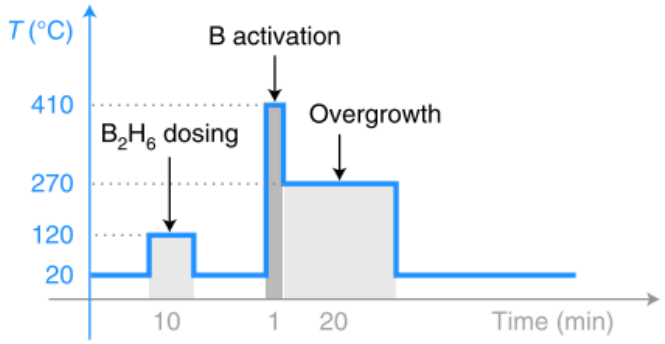
Phosphine sheet density: 1.6 x 10^{14} cm^{-2}

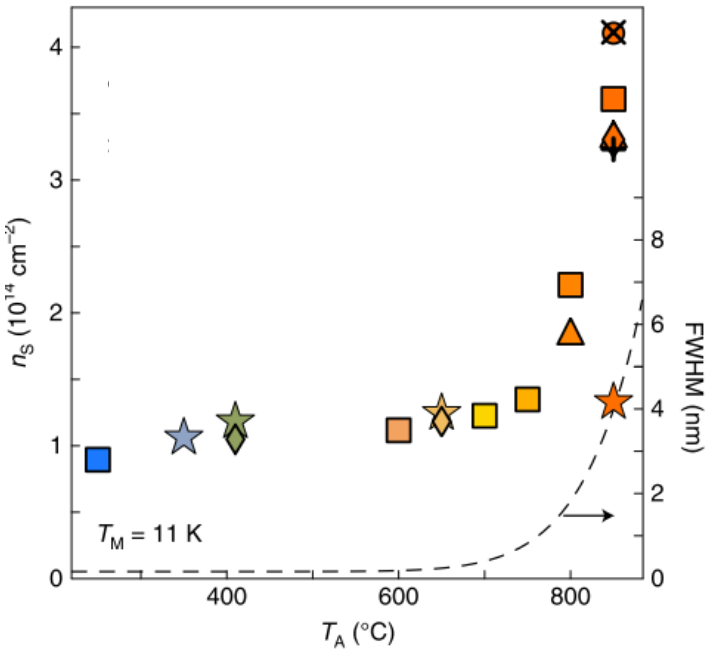


Simulate 2/3 of boron on surface as locked in electrically inactive dimers!

Škereň *et al., Nature Electronics*, 3, 524–530 (2020).
Simmons *et al., Molecular Simulation*, 31, 505-515 (2005).

Incorporation as a function of processing parameters





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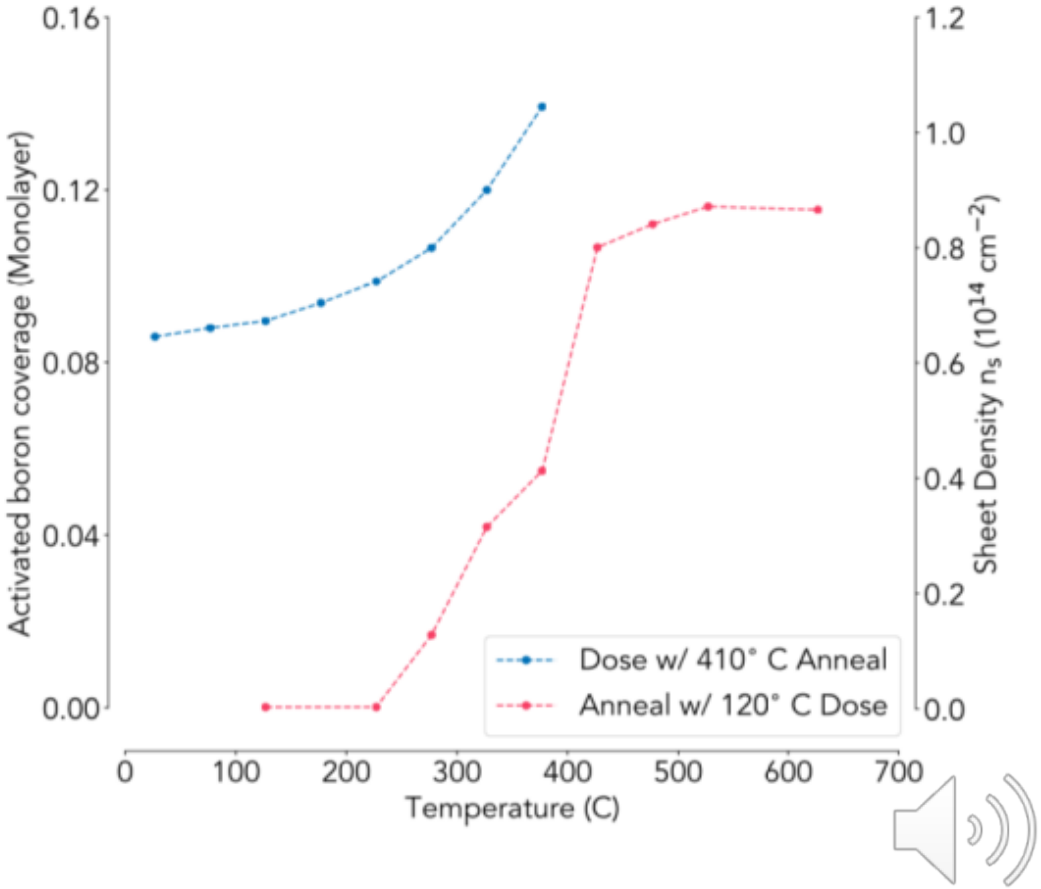
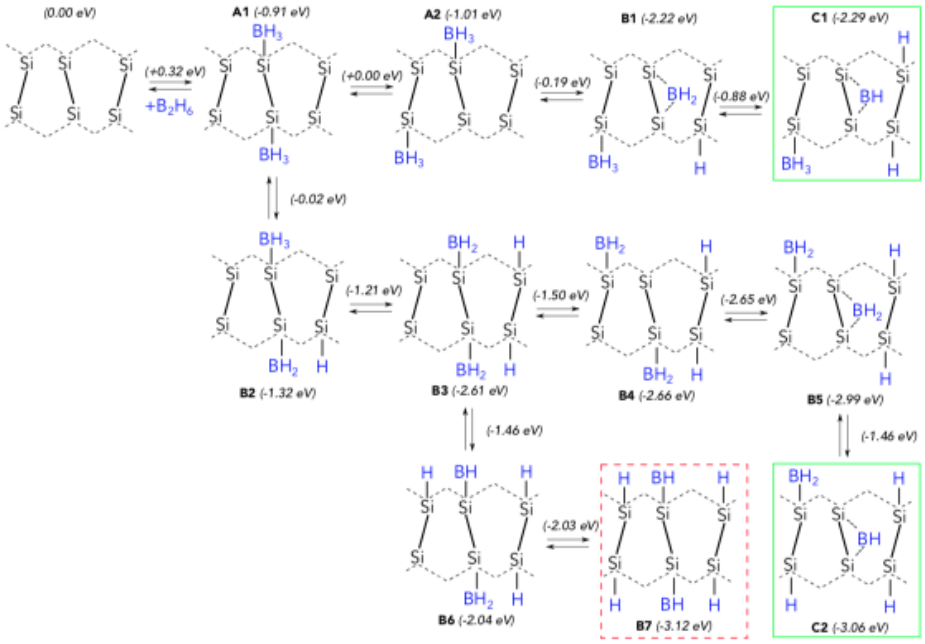


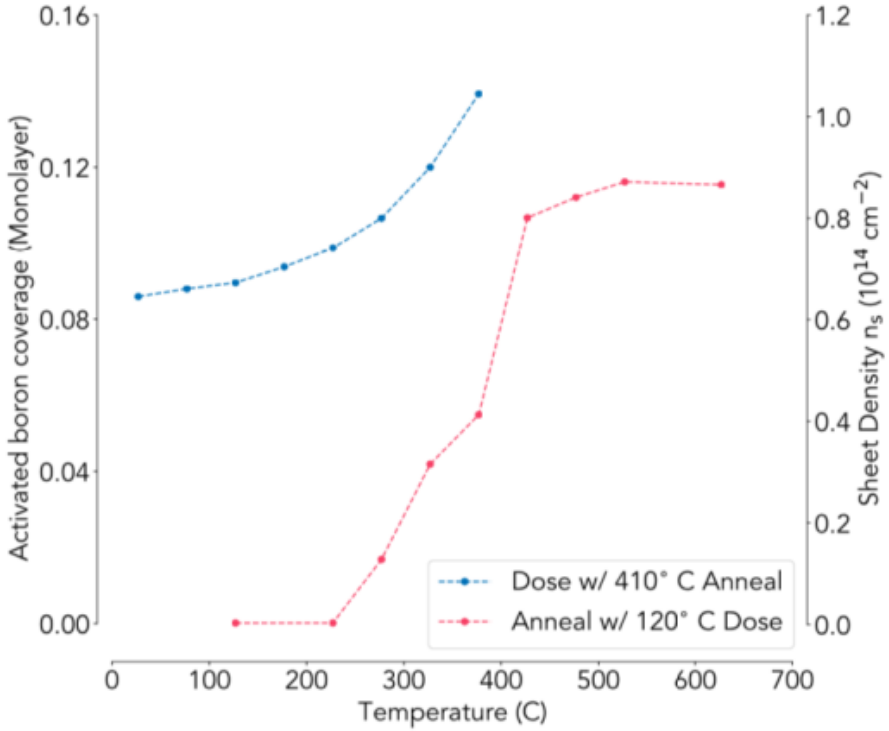
We do *not* model boron dimers breaking apart, which Škereň et al. attribute to rise after 800 °C

Škereň *et al., Nature Electronics*, 3, 524–530 (2020).
Simmons *et al., Molecular Simulation*, 31, 505-515 (2005).

Summary

Dimer nature of diborane limits its usefulness as an atomic precision precursor





For full detail checkout:
https://arxiv.org/abs/2010.00129

Thanks for your attention!
Feel free to reach out with questions at qcampbe@sandia.gov

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This work was supported by the Laboratory Directed Research and Development Program at Sandia National Labs.
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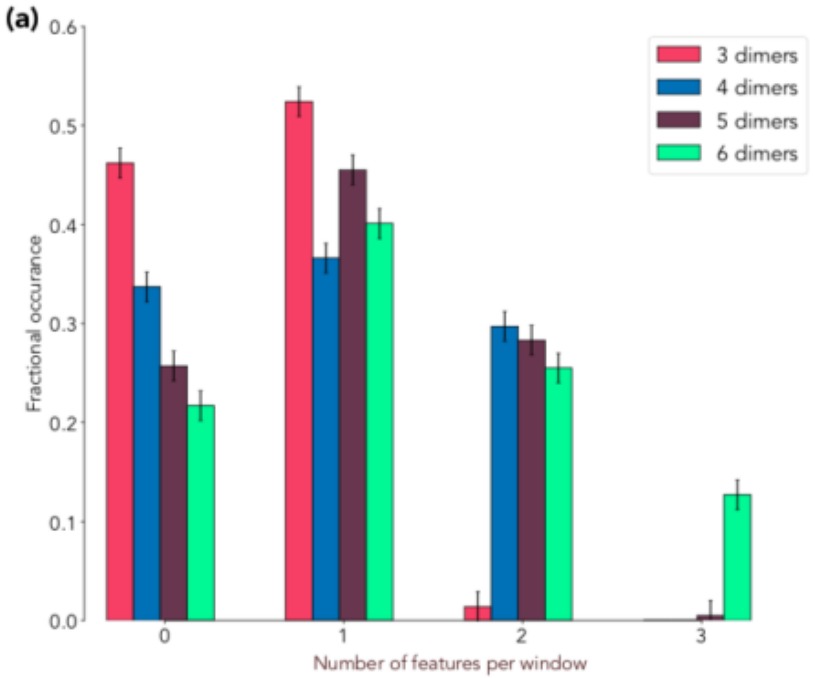
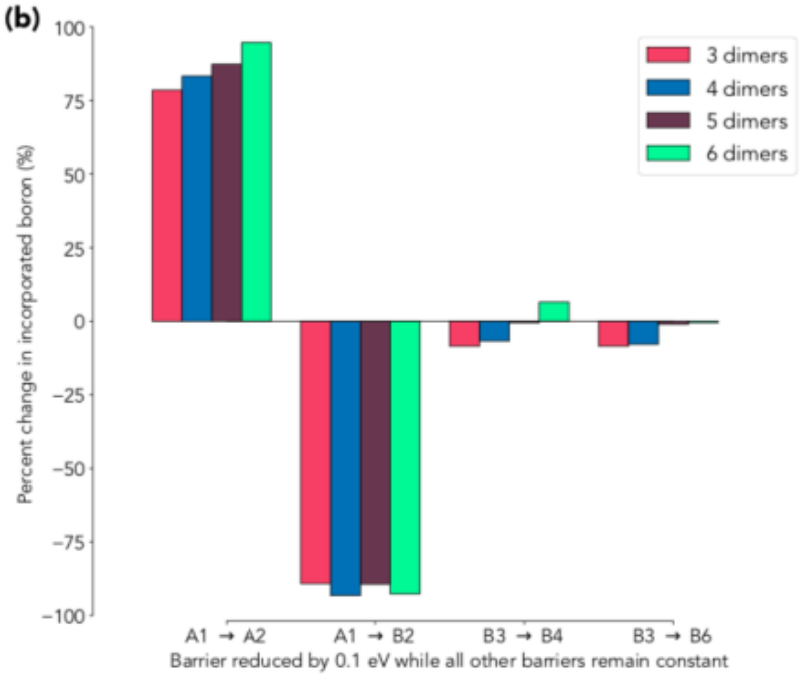
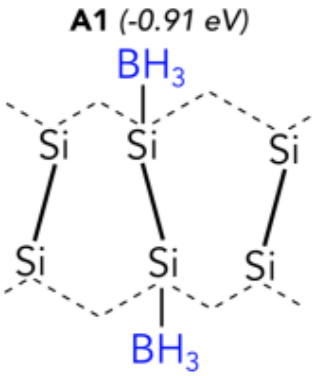
CCR
Center for Computing Research

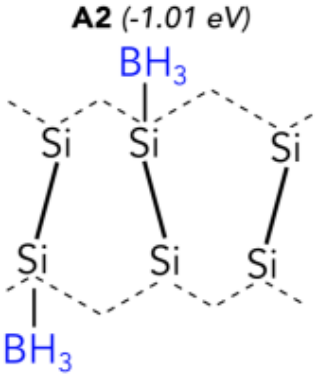
Incorporation in small dimer windows

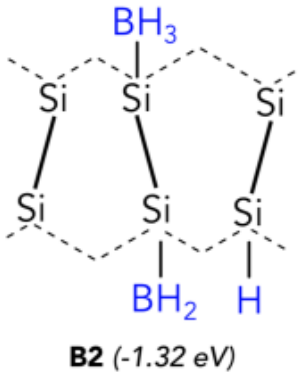
Fed the calculated barriers into a Kinetic Monte Carlo (KMC) model to calculate rates









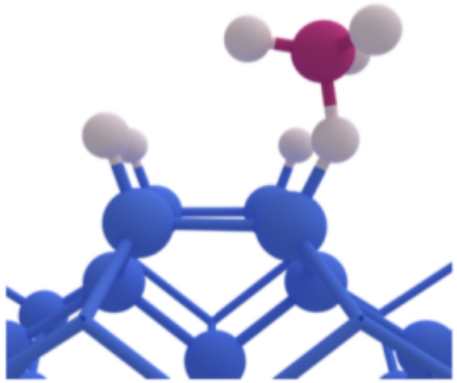


BH_x monomer adsorption

BH_3 adsorption on bare Si

E_a =-1.90 eV

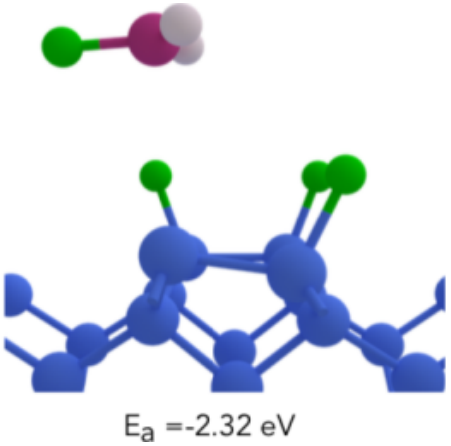
BH_3 adsorption on H-terminated Si



E_a =-0.75 eV

E_a =-3.20 eV

BH_2 adsorption on H-terminated Si



E_a =-2.32 eV

BH_2 adsorption on Cl-terminated Si

BH_x fragments largely not selective versus hydrogen/chlorine resists