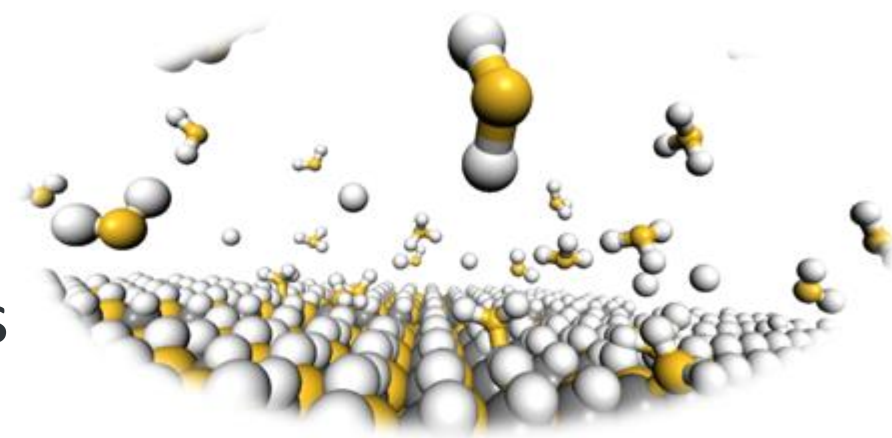
The difference in nucleation of silicon-based materials during PECVD/PEALD for future S-ALD



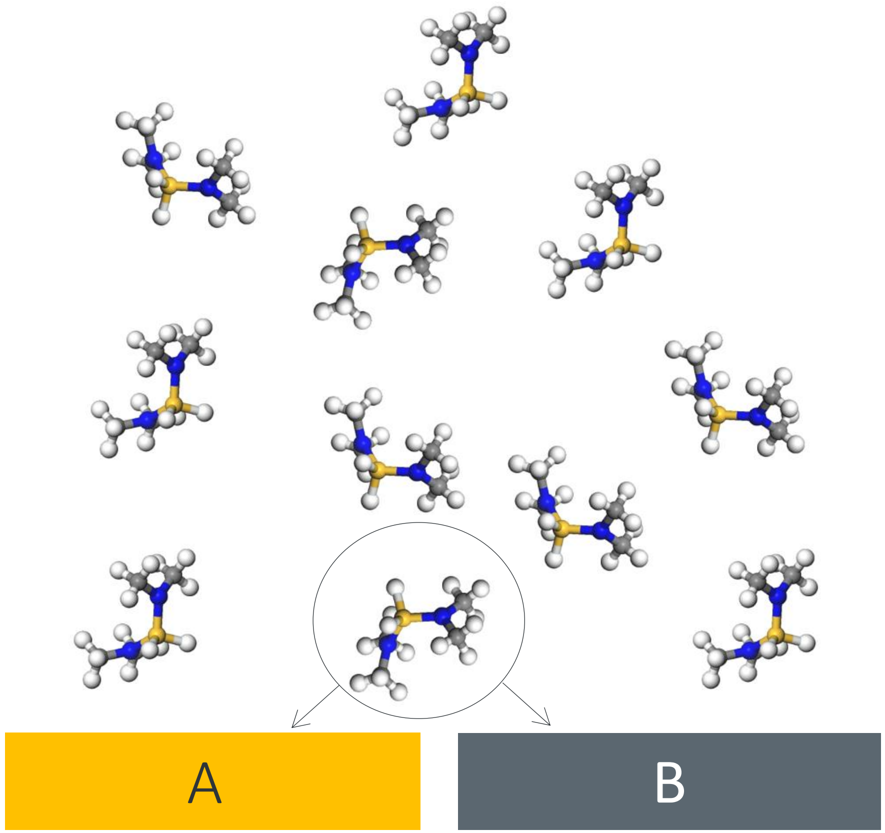
Ekaterina Filatova †
Dr. Simon Elliott †
Dr. Dennis Hausmann ‡

21.04.2017

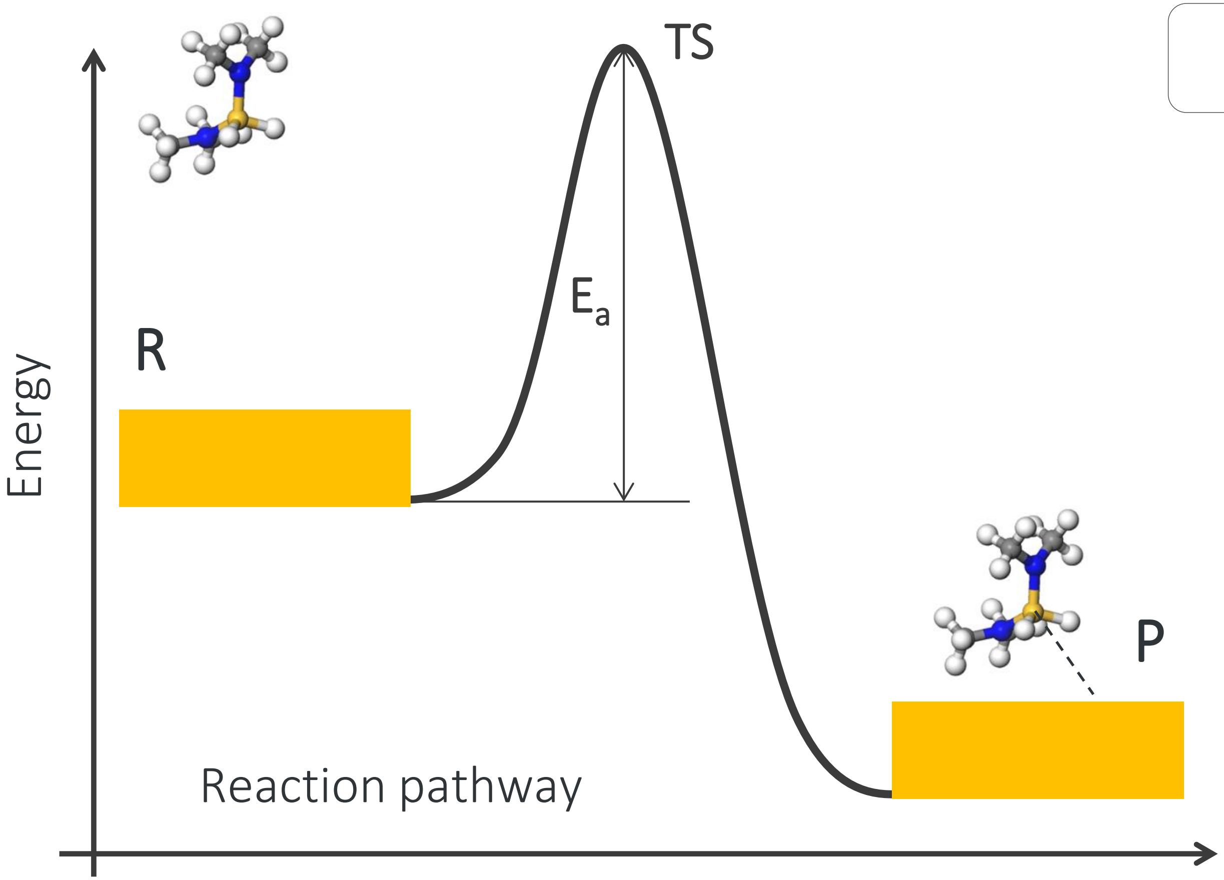
† Tyndall National Institute, University College Cork, Ireland
‡ Lam Research Corporation, Portland, OR, USA

Theoretical modelling
for area selective deposition

Precursor



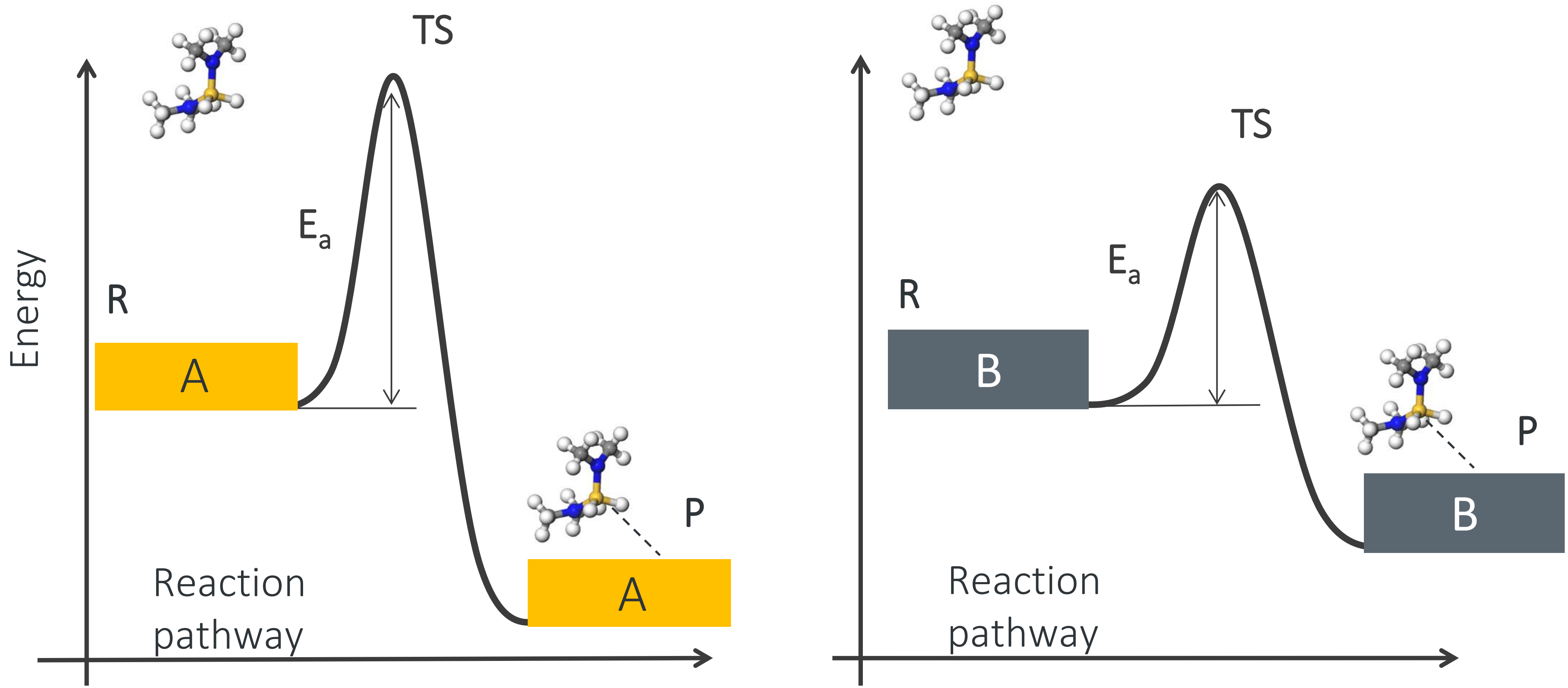
Theoretical modelling for area selective deposition



DFT calculations

R - reactants   TS - transition state   P - products E_a - activation energy

Theoretical modelling for area selective deposition



R - reactants TS - transition state P - products E_a - activation energy

Si-based thin films

- Excellent barrier
- Low-k
- Low wet etch rate

Si-based thin films

(1) SiC

SiO_2

(2)

Si_3N_4

Silane plasma fragments with H-SiC

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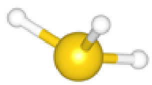
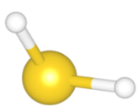
SiC



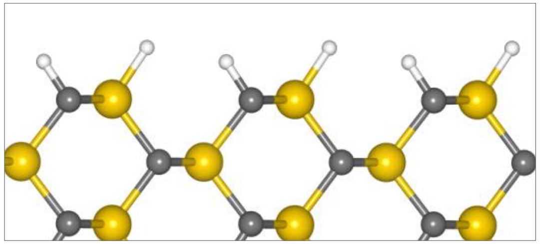
Silyl (SiH_3)



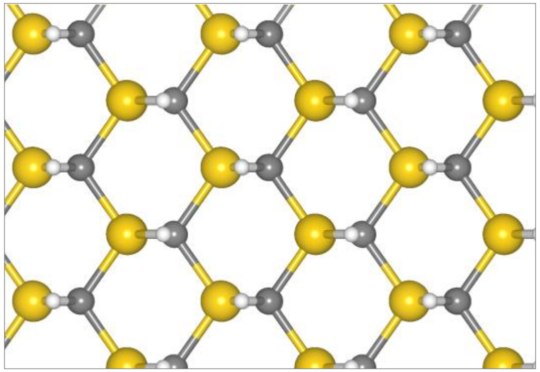
Silylene (SiH_2)

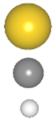
+

(011) 3C H-SiC Side view



(011) 3C H-SiC Top view





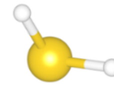
Si
C
H

DFT (VASP)
k-points: 2x2x1
core electrons:
- PAW (projector augmented wave)

valence electrons:
- plane wave basis set with $E_{cut\text{-}off}$=400 eV

energy barriers:
- CI – NEB (5 images, force constant 5) T = 0 K

Silane plasma fragment SiH_2 with H-SiC



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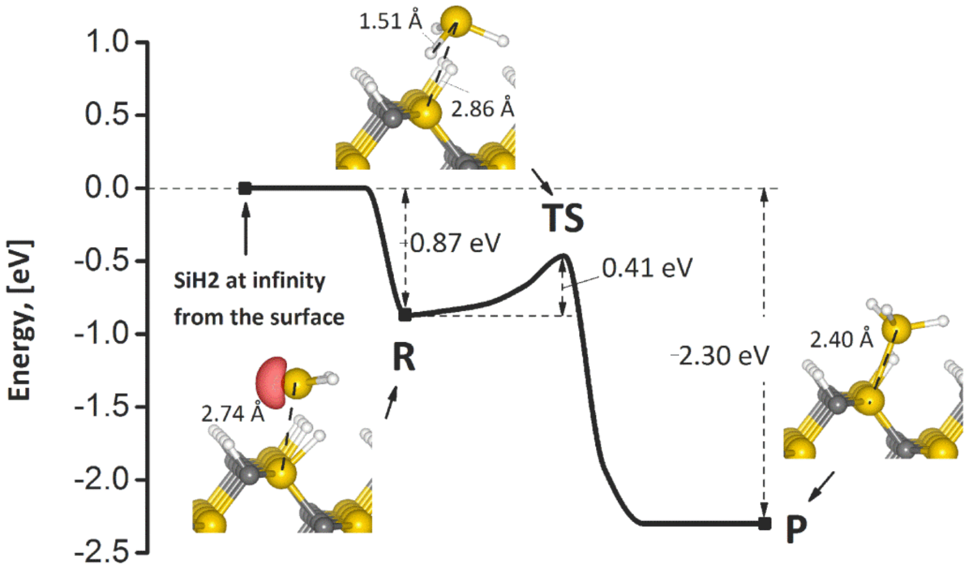
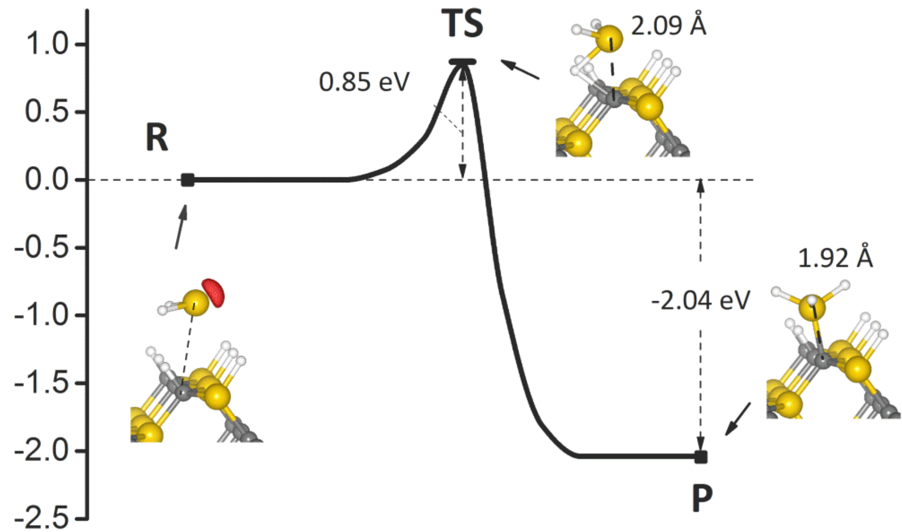
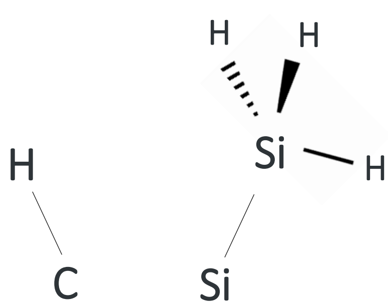
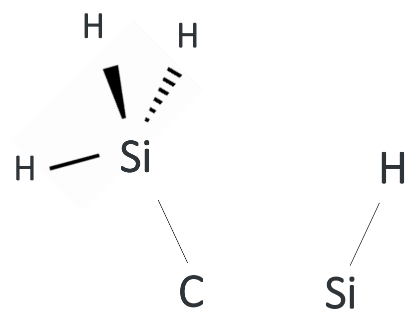
SiC









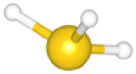
(0 1 1) H-SiC

Si – H

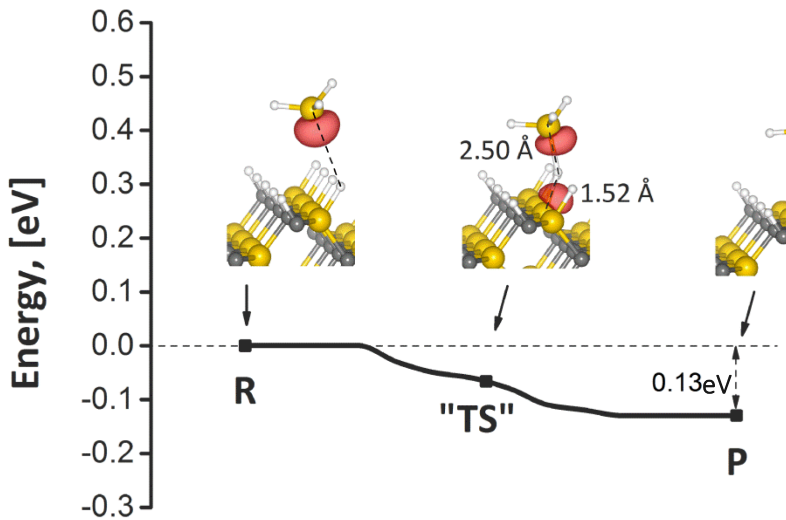
(0 1 1) H-SiC

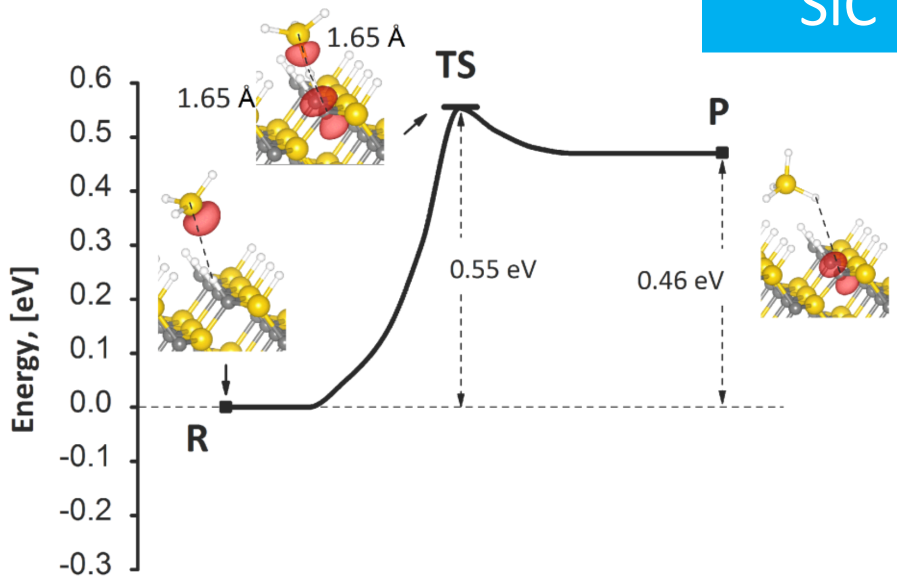
C – H

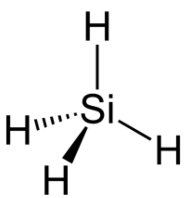
Silane plasma fragment SiH_3 with H-SiC

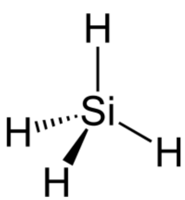


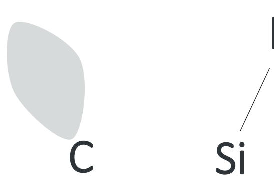
SiC











(0 1 1) H-SiC

Si – H

(0 1 1) H-SiC

C – H

Silane plasma species with H-SiC Summary

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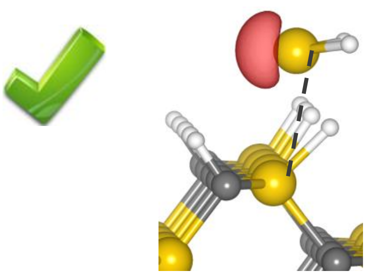
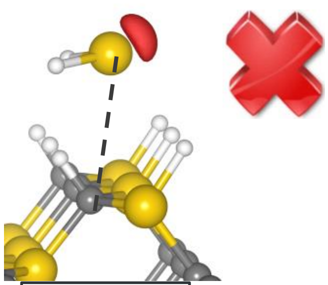
SiC

- Both silyl and silylene show selectivity towards insertion into the Si-H bond, rather than the C-H bond

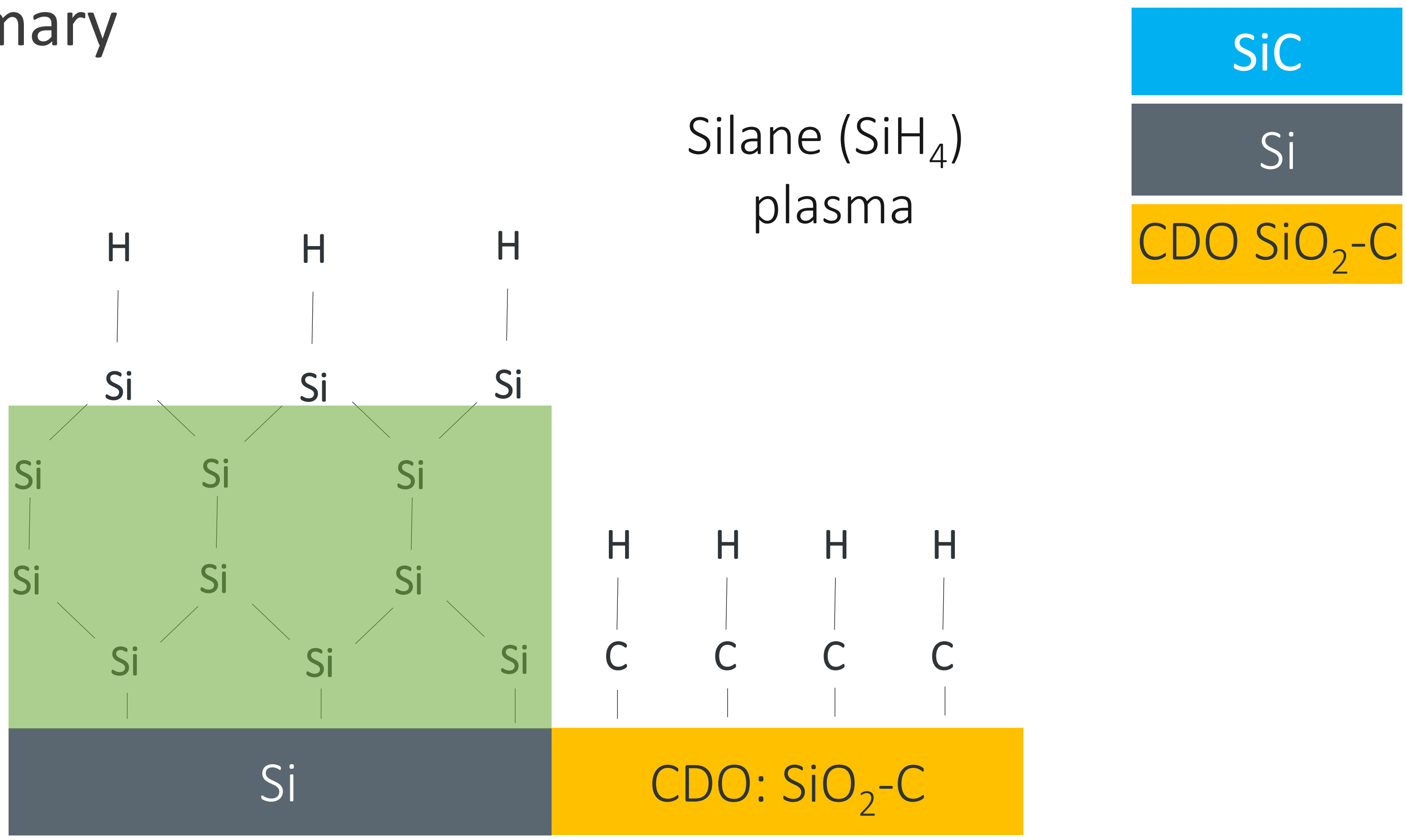


Si – H



C – H

Silane plasma species with H-SiC Summary



Selectivity towards Si

Si-based thin films

(1) SiC

(2) SiO_2

Si_3N_4

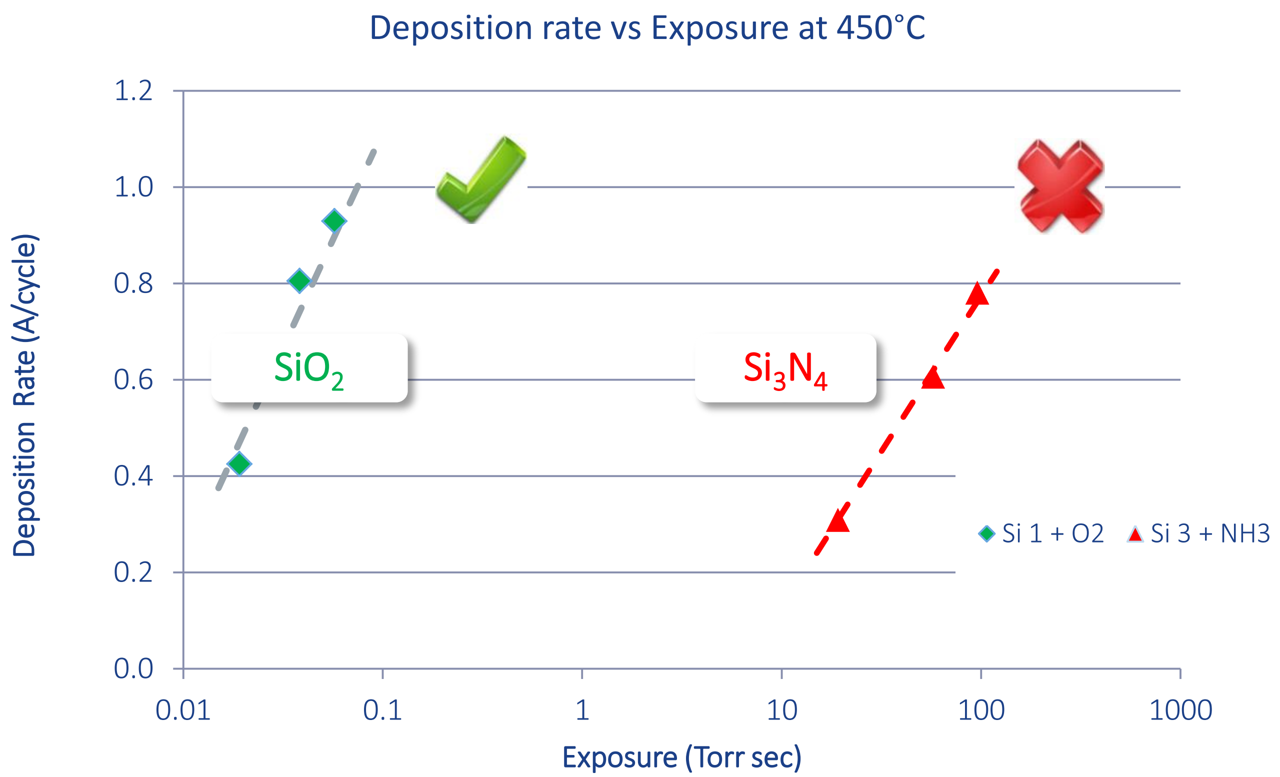
Reactivity of Si_3N_4 versus SiO_2

SiO_2

Si_3N_4

Why is the Si_3N_4 reaction slower?

How the problem can be solved?

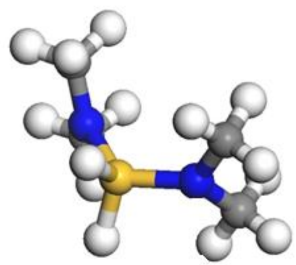


Reactivity of Si_3N_4 versus SiO_2

SiO_2

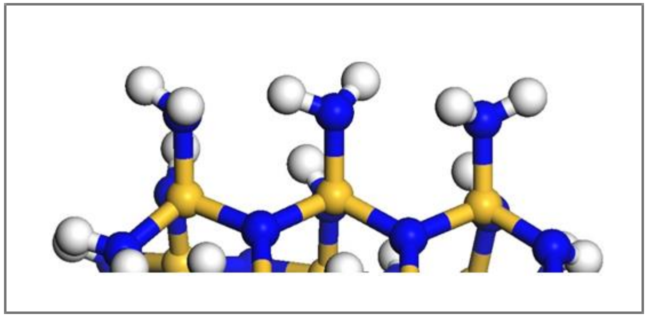
Si_3N_4

$SiH_2(NMe_2)_2$

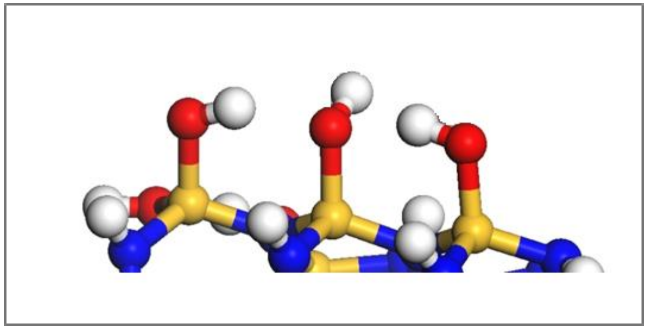


+

Side view

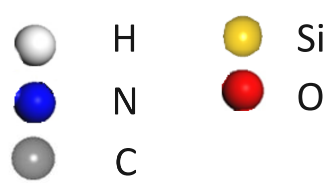


NH_2 surface model for Si_3N_4



OH surface model for SiO_2

DFT (TURBOMOLE)
- BP86/TZVPP
- *T* = 0K



Reactivity of Si_3N_4 versus SiO_2

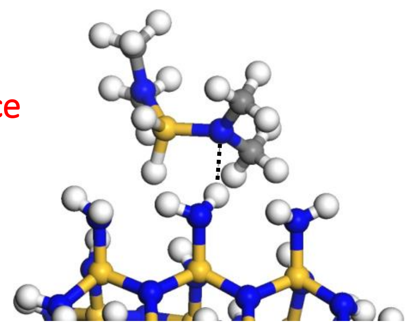
SiO_2

Si_3N_4

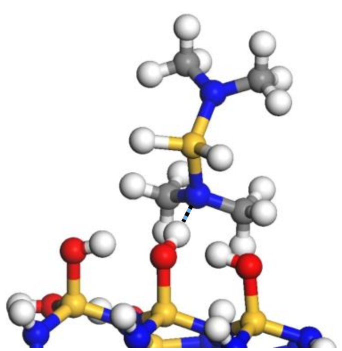
Removing rigid N-H will accelerate ALD reaction

bound precursor

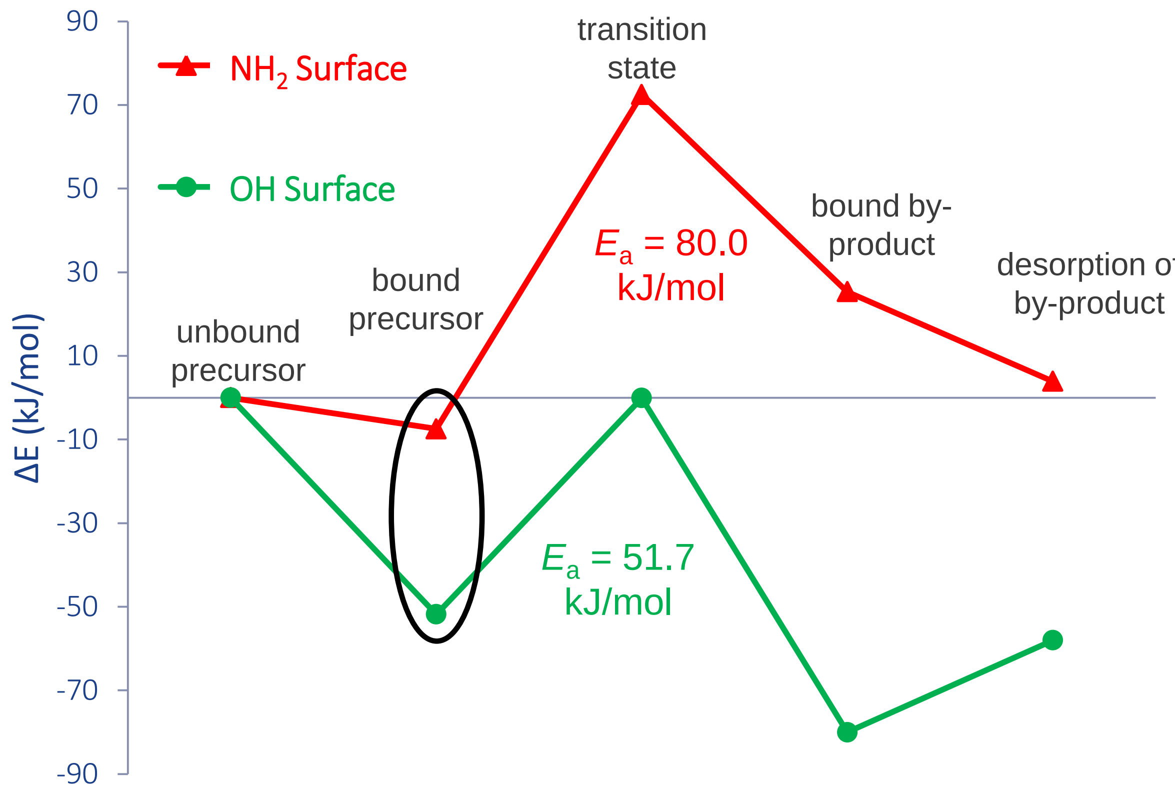
NH_2 surface model for Si_3N_4



OH surface model for SiO_2



H N C Si O

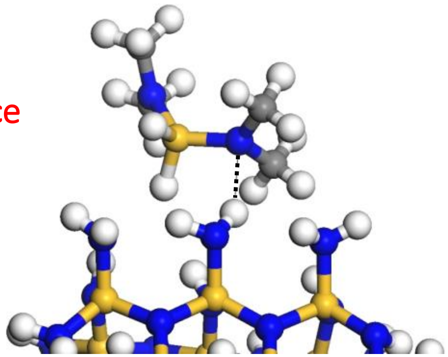


C. M. Murray *et al.*, ACS *Appl. Mater. Interf.* **6**, 10534 (2014)

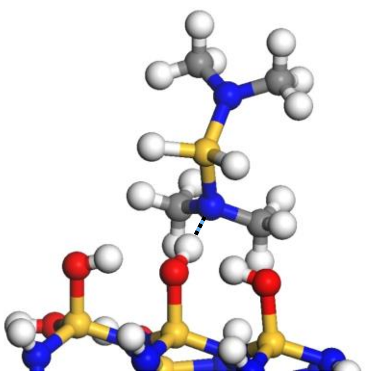
C.K. Ande *et al., J. of Phys.Chem.Letters*, **6**, 3610-3614, (2015)

Reactivity of Si_3N_4 versus SiO_2 Summary

NH$_2$ surface model for Si_3N_4



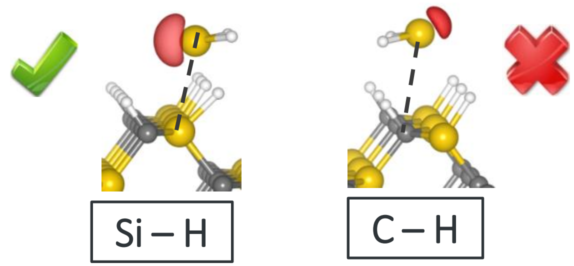
OH surface model for SiO_2



- Si_3N_4 reaction is slower due to N-H rigidity
- Removing rigid N-H will accelerate ALD reaction

Silicon-based materials during PECVD/PEALD for future S-ALD

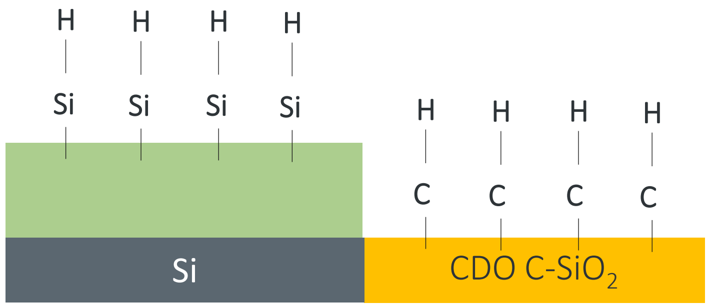
SiC



- Selectivity towards Si-H bond

CDO C-SiO_2

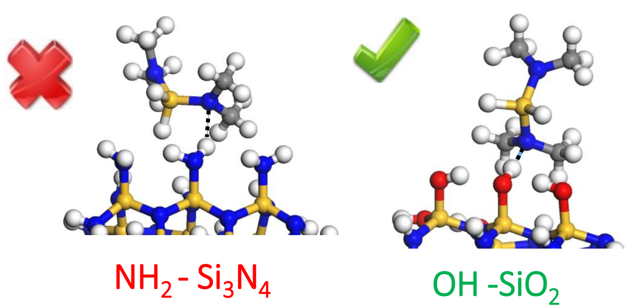
Si



- Selectivity towards Si

SiO_2

Si_3N_4



- Si_3N_4 reaction slower due to N-H rigidity
- Removing rigid N-H accelerate ALD reaction

Acknowledgements

Lam® RESEARCH

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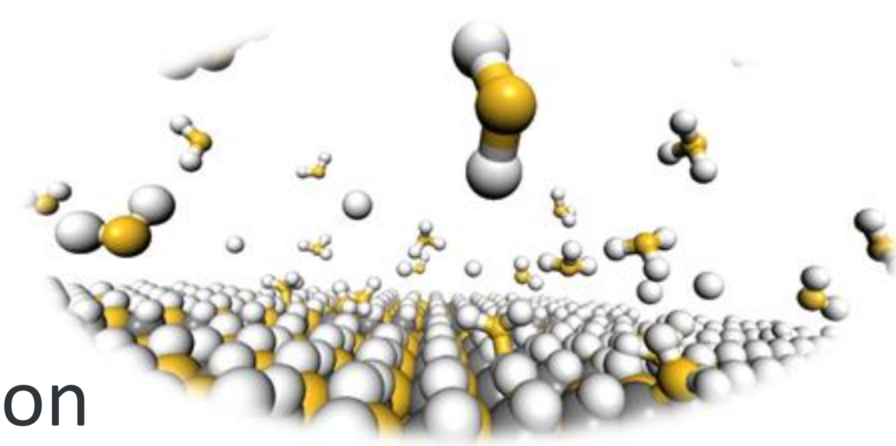
ICHEC
Irish Centre for High-End Computing



The difference in nucleation of silicon-based materials during PECVD/PEALD for future S-ALD

Contact email:
ekaterina.filatova@tyndall.ie

Ekaterina Filatova †
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† Tyndall National Institute, University College Cork, Ireland
‡ Lam Research Corporation, Portland, OR, USA