H_2 in Oxides: Implications for Radiation Response

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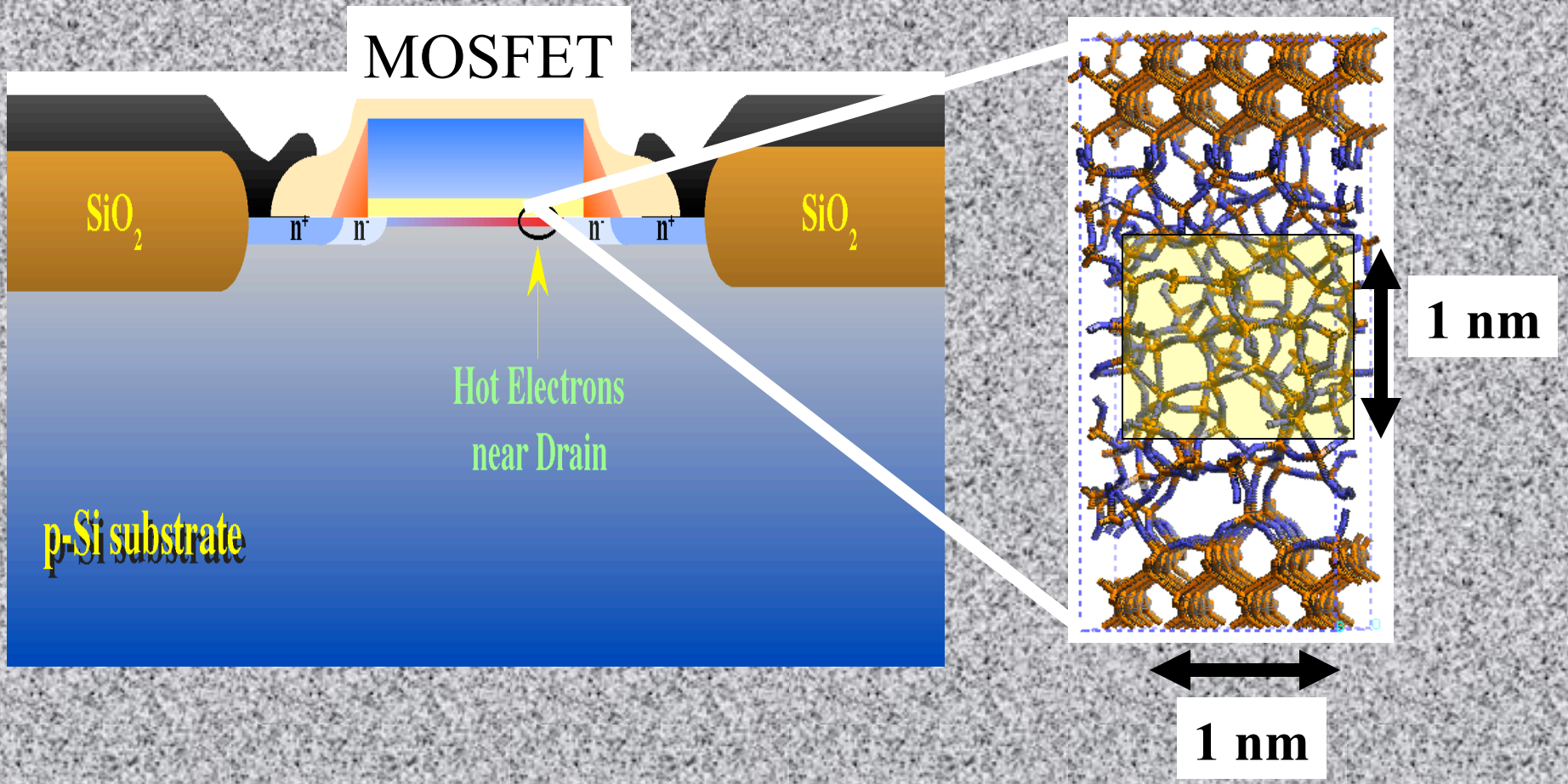
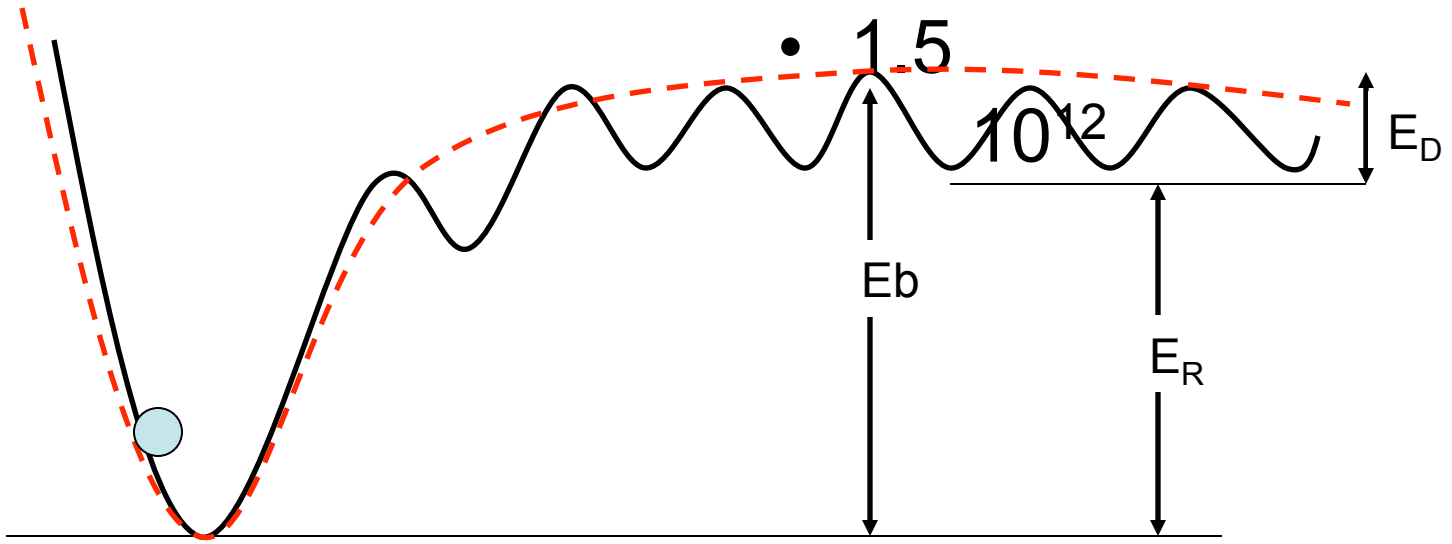
Microscopic modeling of oxides



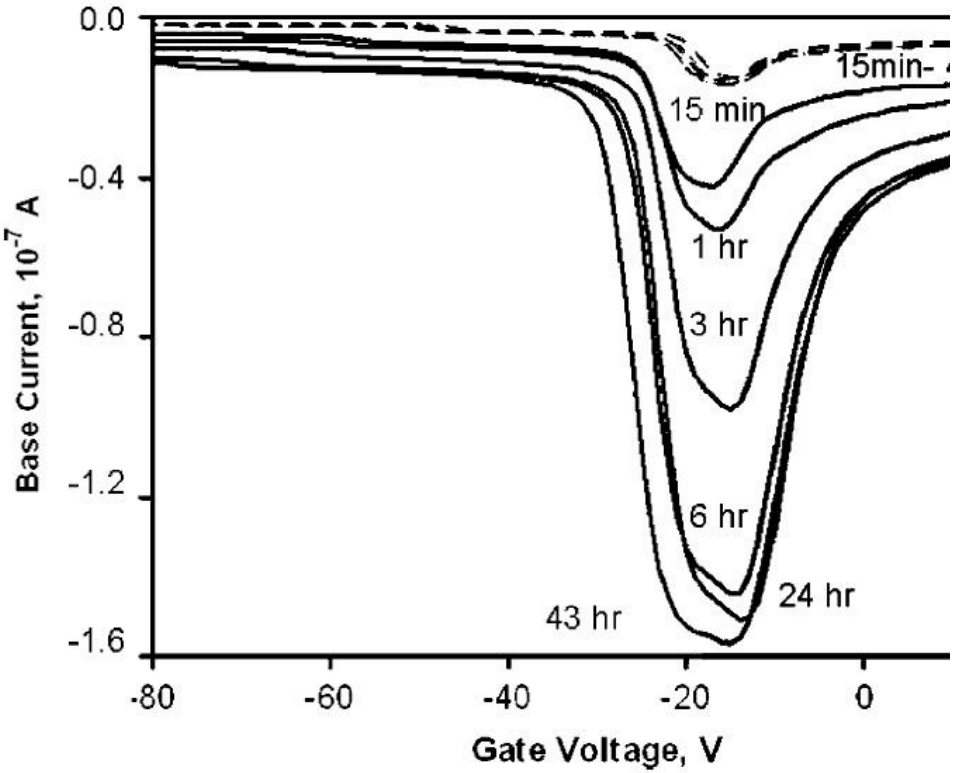
Reaction Time

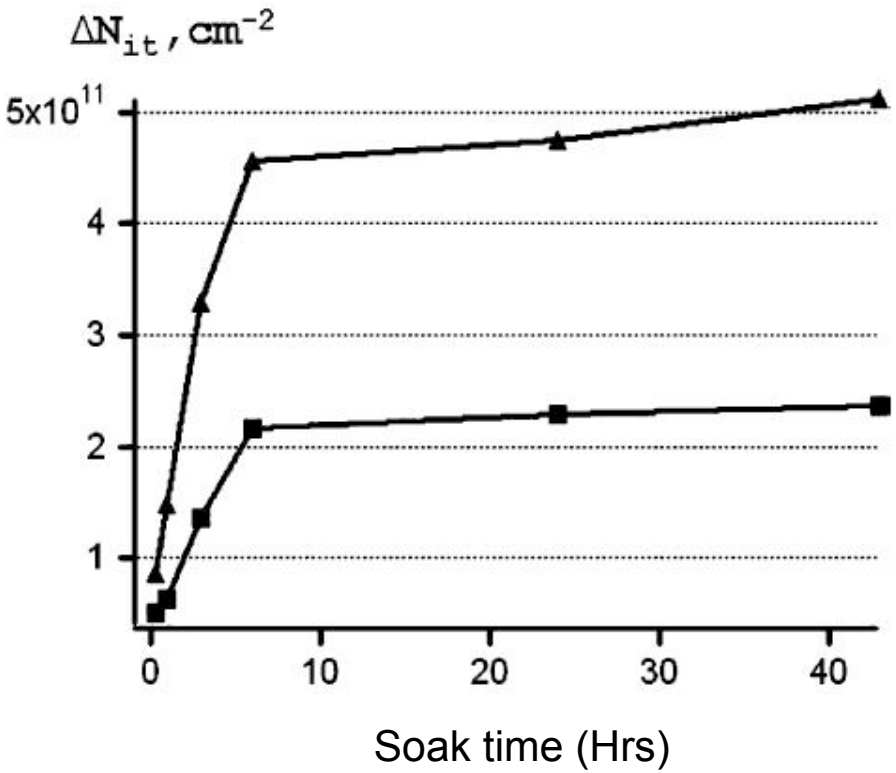
- time ~ [1 / f] $e^{Eb/kT}$
- f ~ 10^{14} Hz
- kT_{300K} ~ 0.025 eV

Eb(eV)	time(s)
0.5	10^{-6}
1	10^{3}
1.5	10^{12}



H_2 Soaking Experiments

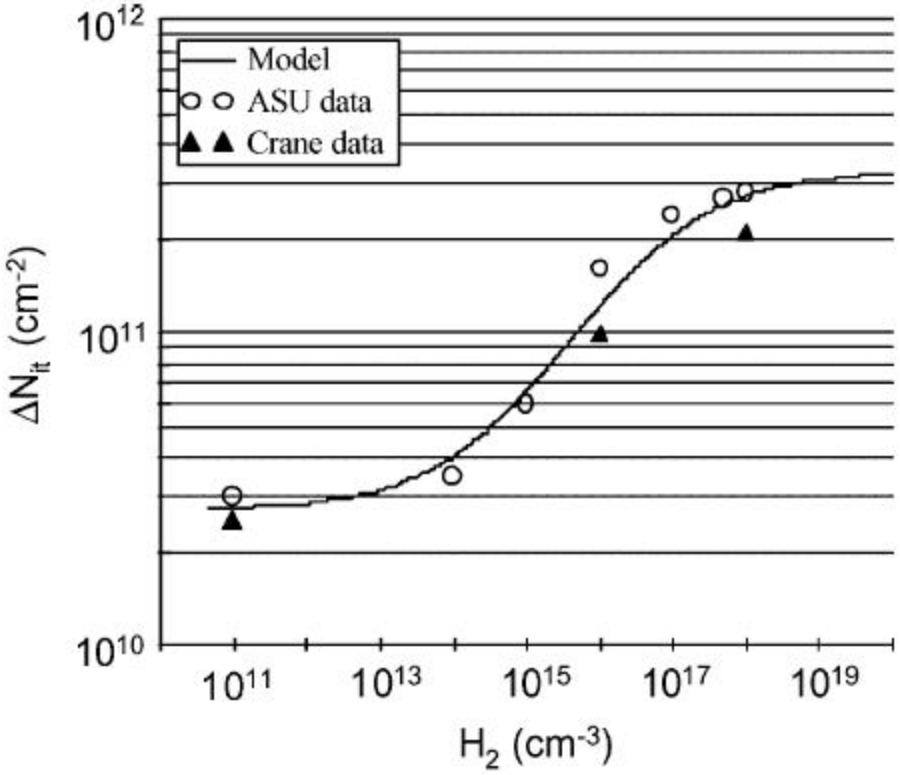




ΔN_{it} after minutes of irradiation

Reaction Models

- Chen et. al. IEEE Trans. Nuc. Sci. 2007
  - $H_2 + 2\,D \leftrightarrow 2\,DH$
- $DH + hole \rightarrow D + H^+$

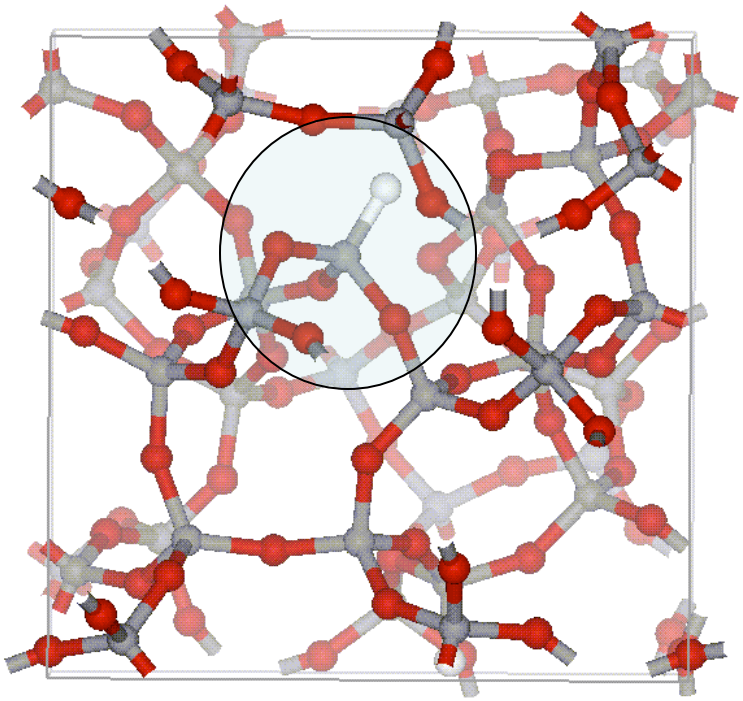


$$\Delta N_{it} = N_{DH} + K_1 (N_{H2})^{1/2} / (1 + K_2 (N_{H2})^{1/2})$$

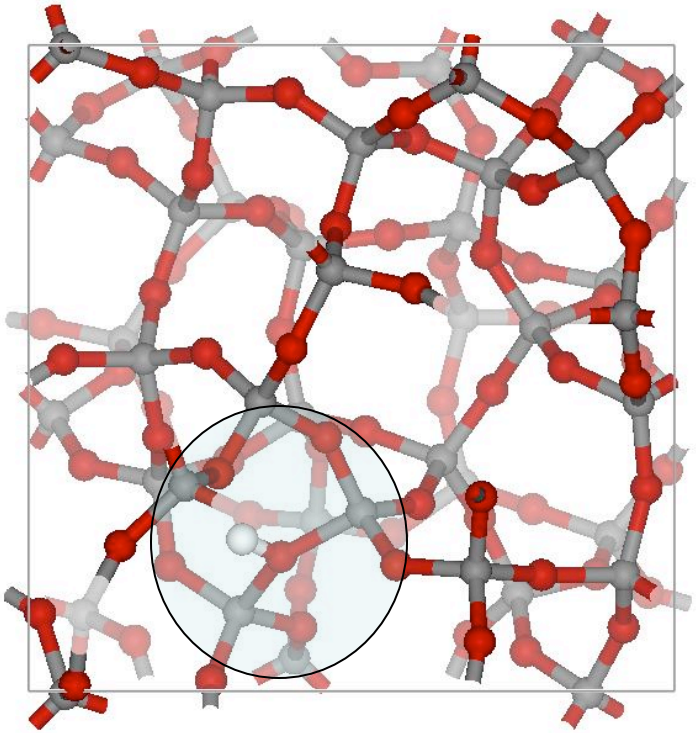
What is D ?

- D = isolated defect center
- D ~ E' ?
- 2000 – Afanasev and Stesmans
  - E' = neutral isolated silicon dangling bond

DH + hole → D + H^+



DH model

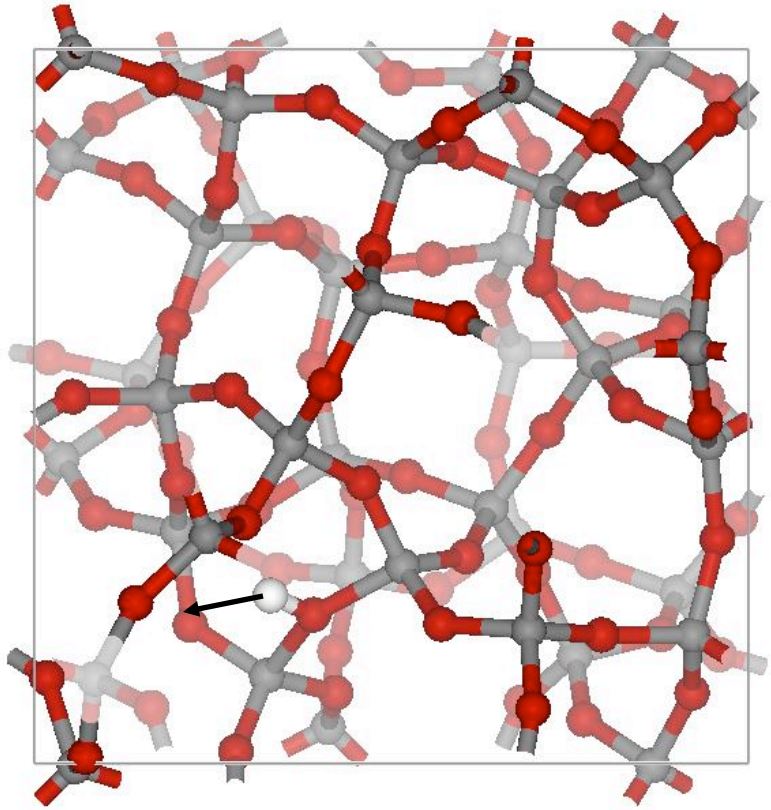


Interstitial H^+

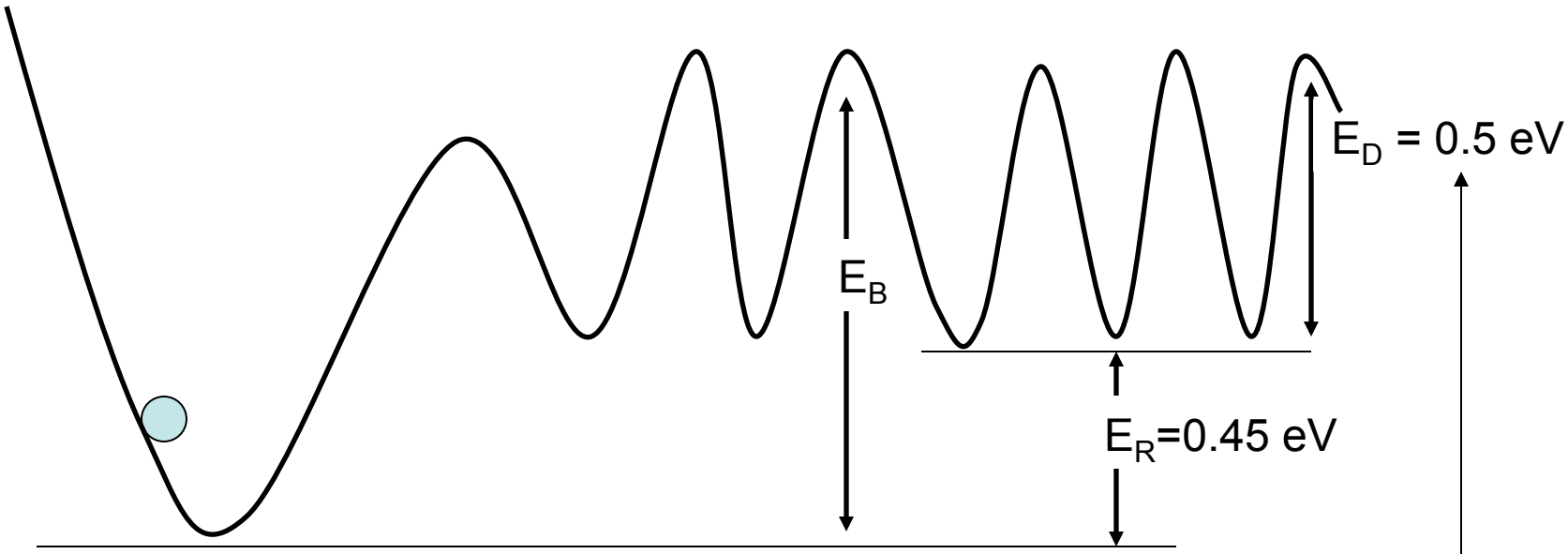
	Reaction Energy (eV)
Present Work	0.45 +/- 0.15

Interstitial Diffusion

- H^+ in oxides
- Barrier: E_b ~ 0.5 eV
  - Theory: Pasquarello et al PRL 2006
  - Experiment: Devine and Herrera 2001



H^+ Release Reaction

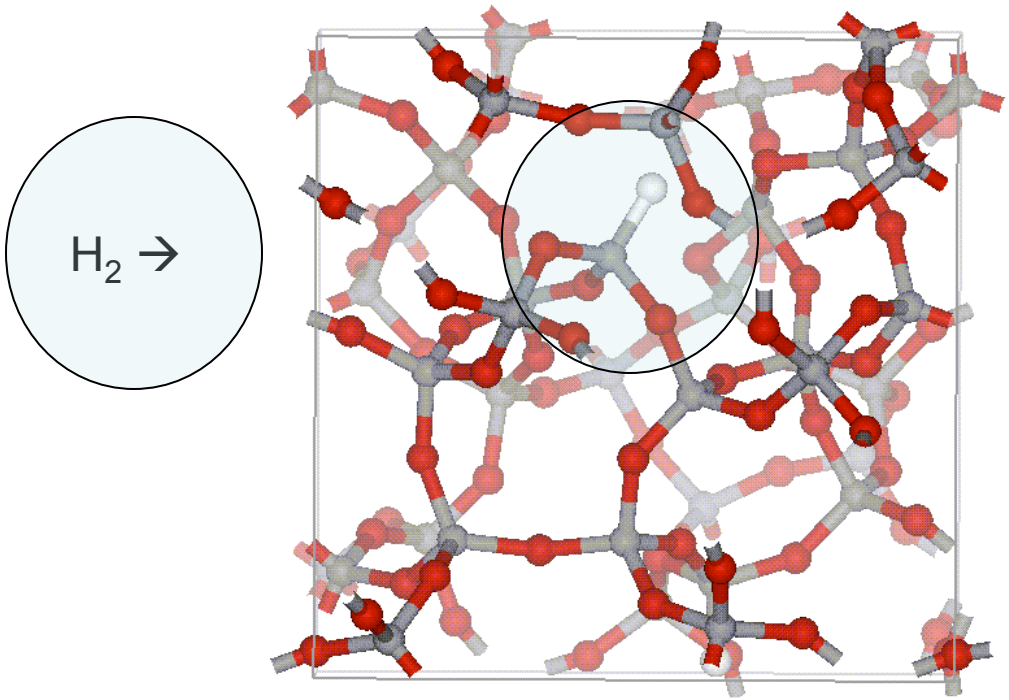


	Barrier (eV)
Interstitial H+ Pasquarello	0.5

Reaction Barrier ~ 0.95 +/- 0.15 eV
Reaction time ~ 10^3 sec ~ 20 min

← A little too long !!!!

$2D + H_2 \rightarrow 2DH$

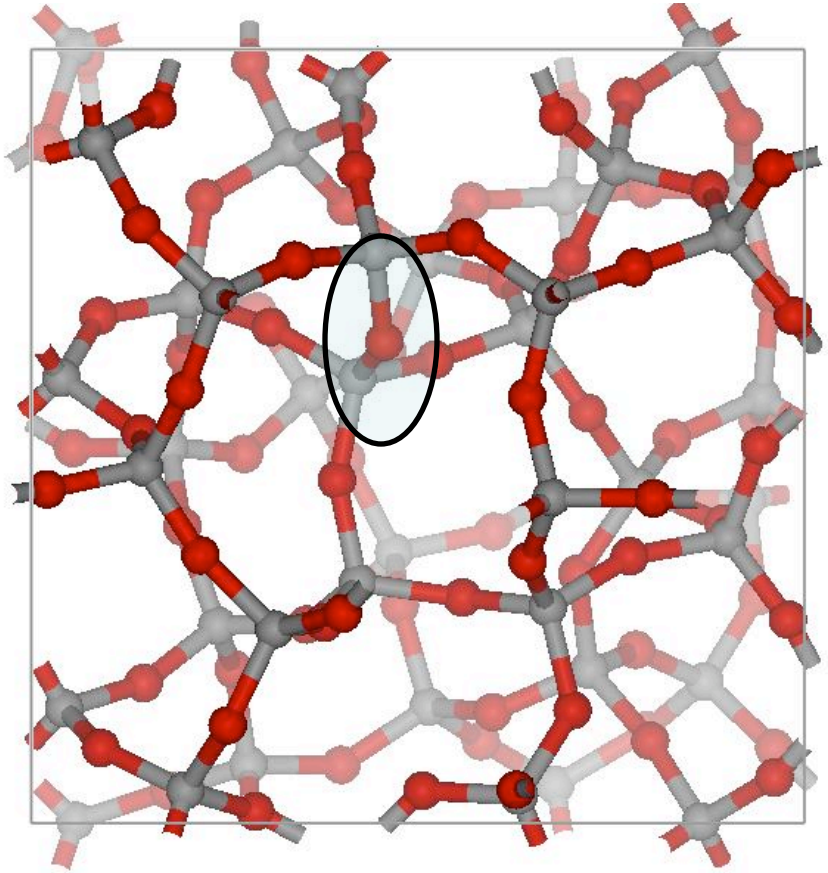


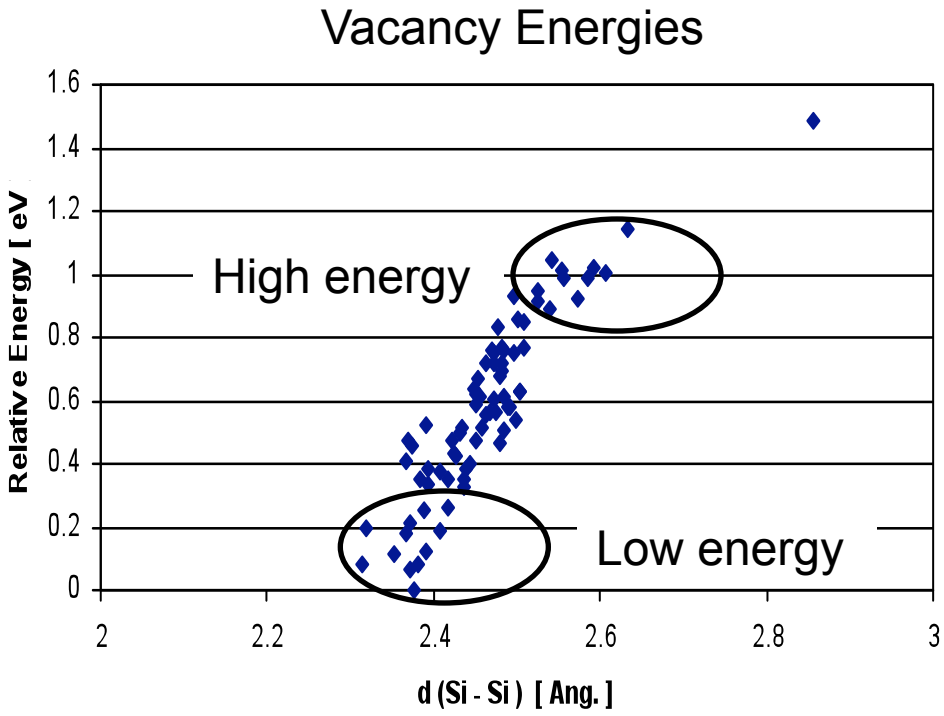
- $2D + H_2 \rightarrow 2DH$
- $E_R > 4$ eV
- All D → DH
- No D during H_2 soak

New Model Needed

- Initial Model
  - H_2 + 2 D → D H
  - DH + hole → D + H^+
  - D = isolated dangling bond
- New Model
  - D = Oxygen Vacancy

Oxygen Vacancies

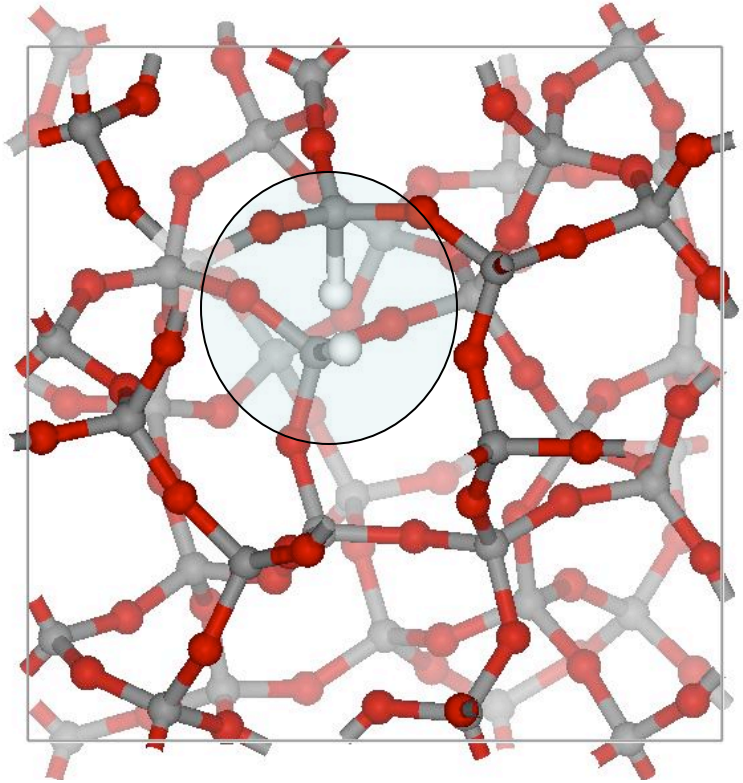




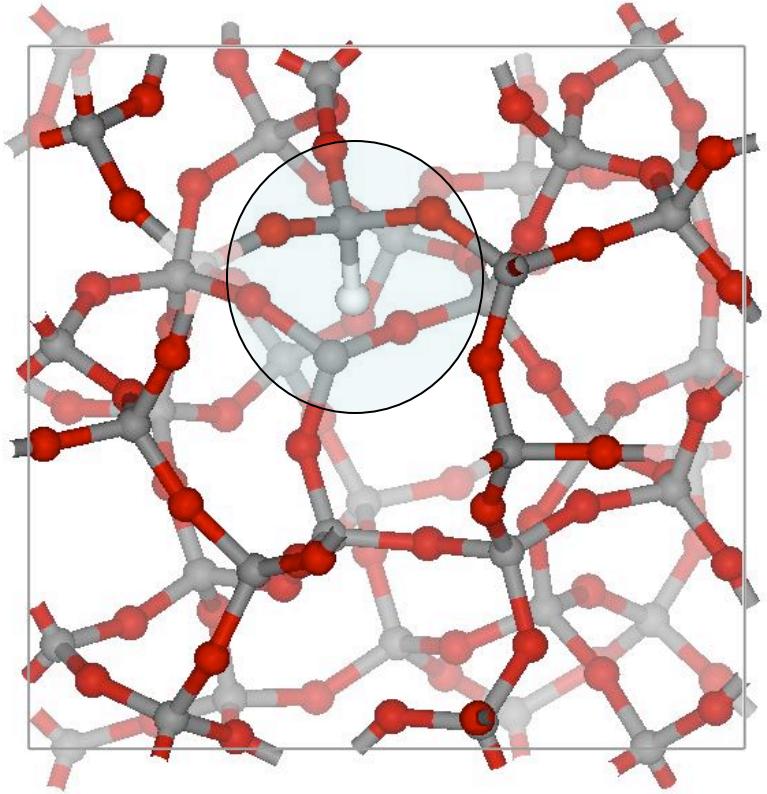
$T \sim 1200\ K$

$N_L / N_H \sim e^{1eV/kT} \sim 10^4$

Hydrogenated Vacancy Models

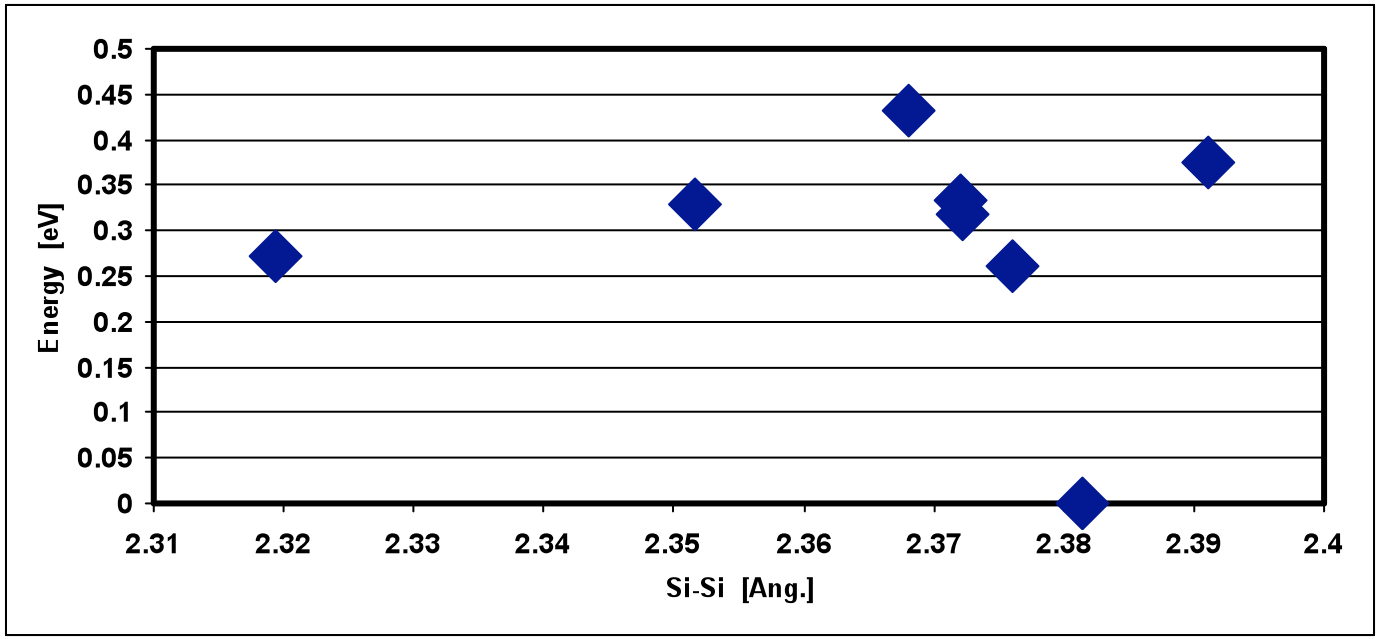


[SiHHSi]$^{+}$



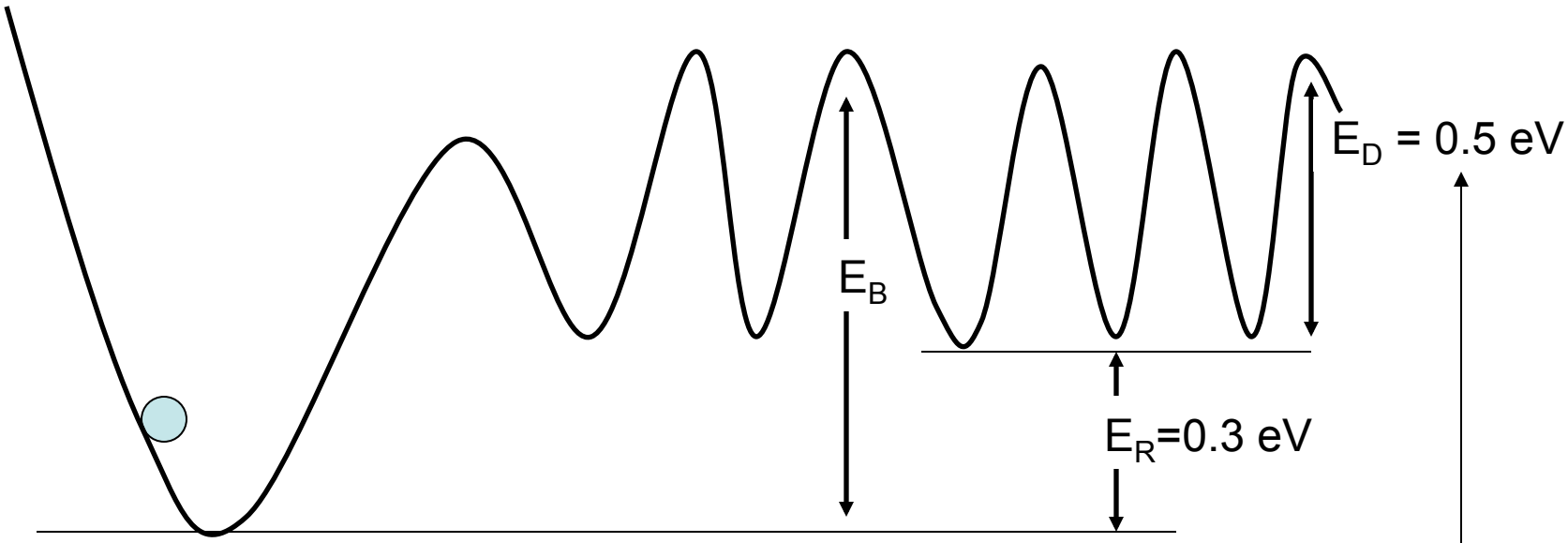
[SiHSi]

$[Si\text{-}HH\text{-}Si]^+ \rightarrow [SiHSi] + H^+$



	Reaction Energy (eV)
Present Work	0.3 +/- 0.1
Blochl, Quartz	0.2

H^+ Release Reaction



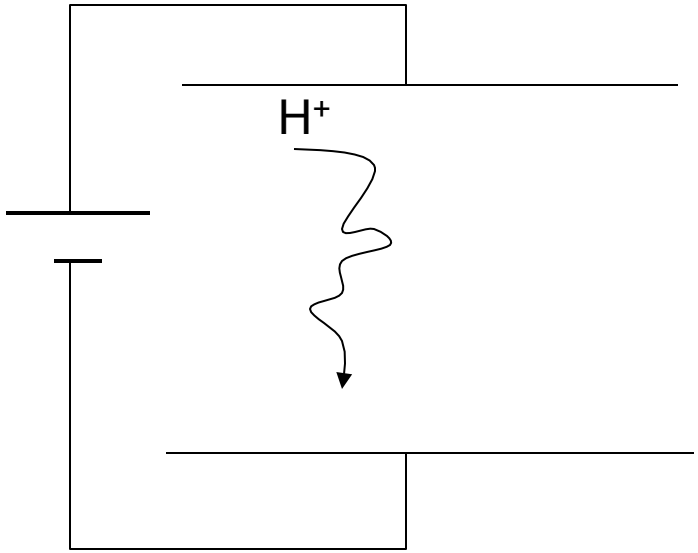
Reaction Barrier ~ 0.8 +/- 0.1 eV
Reaction time ~ 10 sec

$[SiHSi]^+ \rightarrow [SiSi] + H^+$
Reaction Barrier ~ 0.65 +/- 0.1 eV
Reaction time ~ 10^{-3} sec

	Barrier (eV)
Interstitial H+ Pasquarello	0.5

Proton MOS Memory

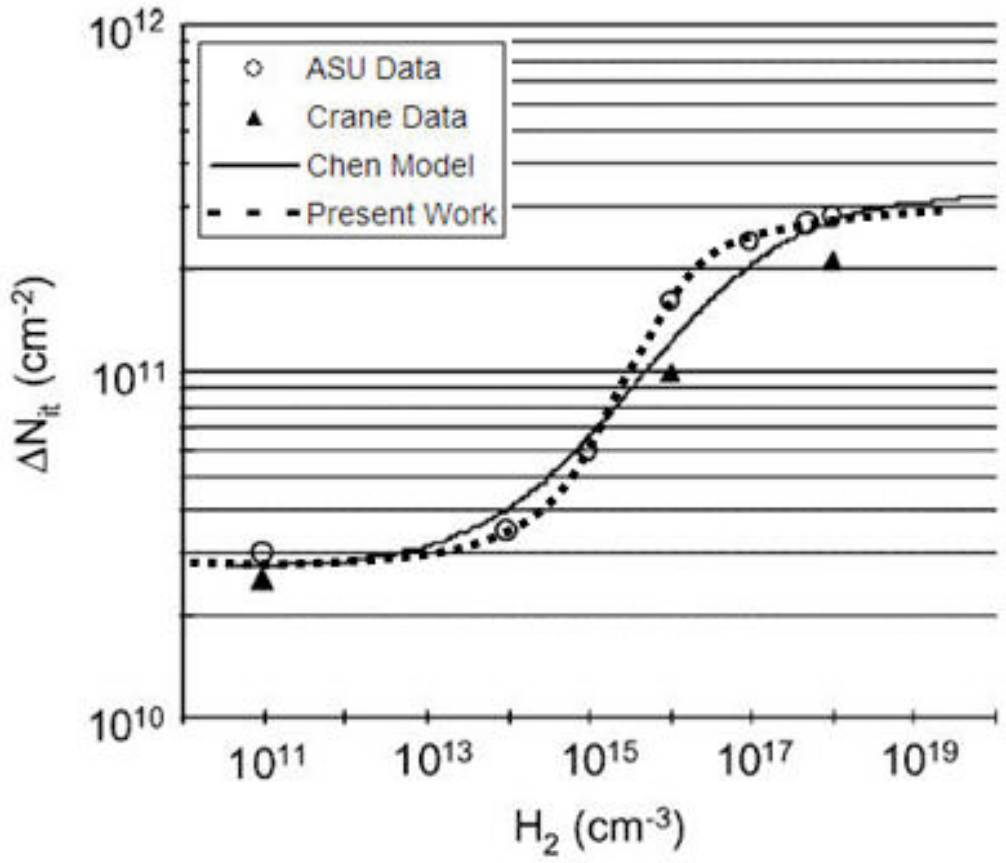
- Vanheusden et al Nature 1997
- H^+ release from vacancies



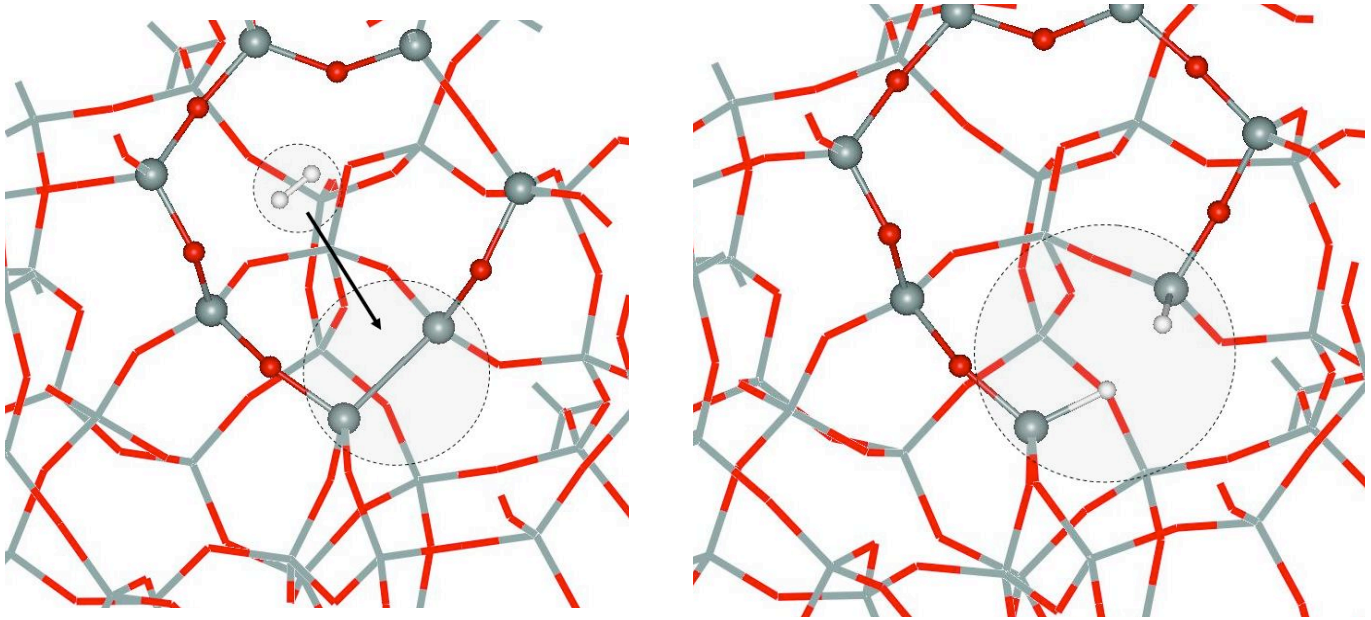
Reaction Models

- Chen et. al. IEEE Trans. Nuc. Sci. 2007
  - $H_2 + 2\ D \leftrightarrow 2\ DH$
  - $DH + hole \rightarrow D + H^+$
  - $\Delta N_{it} = N_{DH} + K_1 (N_{H2})^{½} / (1 + K_2 (N_{H2})^{½})$
- New Reaction:
  - $H_2 + V \leftrightarrow$ (Si-H H-Si)
  - (Si-H H-Si) + hole $\rightarrow$ (Si-H-Si) + H^+
  - $\Delta N_{it} = N_{VH} + K_1 N_{H2} / (1 + K_2 N_{H2})$

Fitting Data

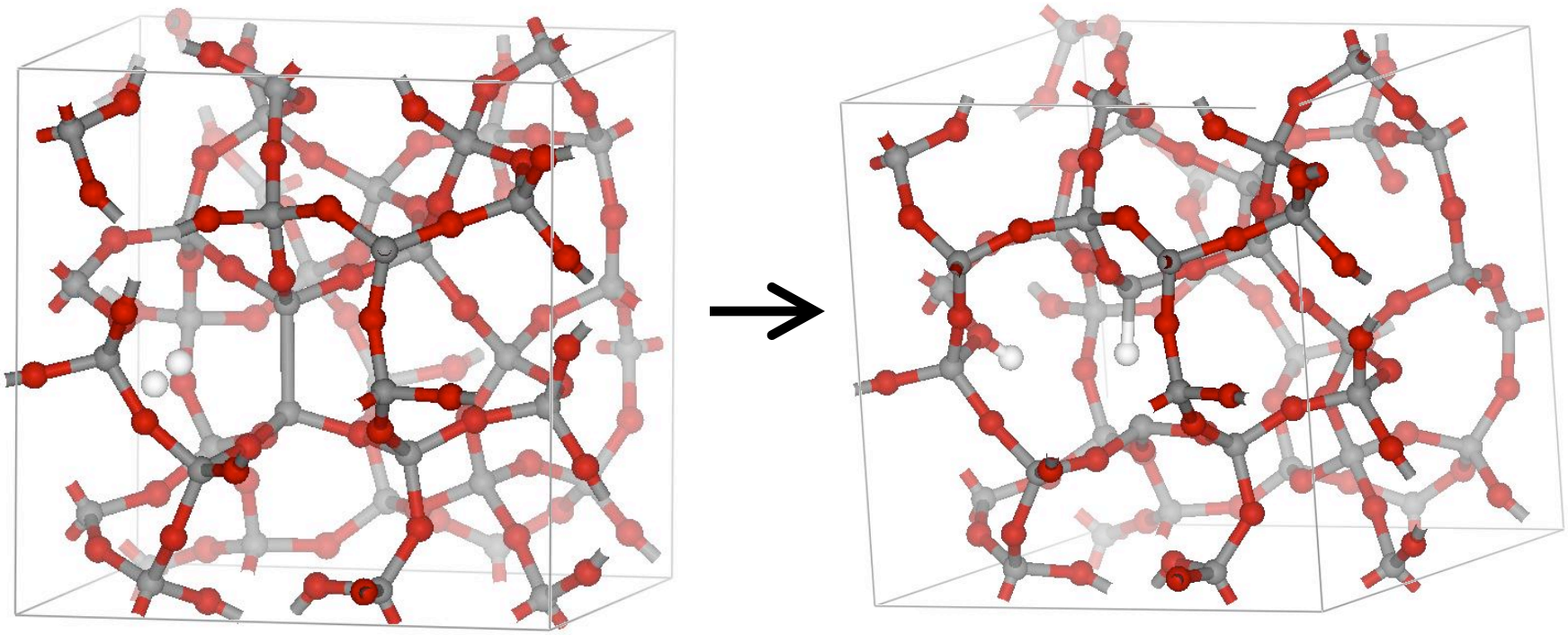


H_2 soaking revisited



- Local Barrier: E_b = 0.95 +/- 0.05 eV

$$H_2 + V^+ \rightarrow VH + H^+$$



Future Work

- More DFT calculations
  - Reduce error bars
- Develop new rate equations
  - Fit to H_2 soaking data