ATOMIC-SCALE THEORY OF RADIATION-INDUCED PHENOMENA

OVERVIEW OF THE LAST FIVE YEARS

AND NEW RESULTS

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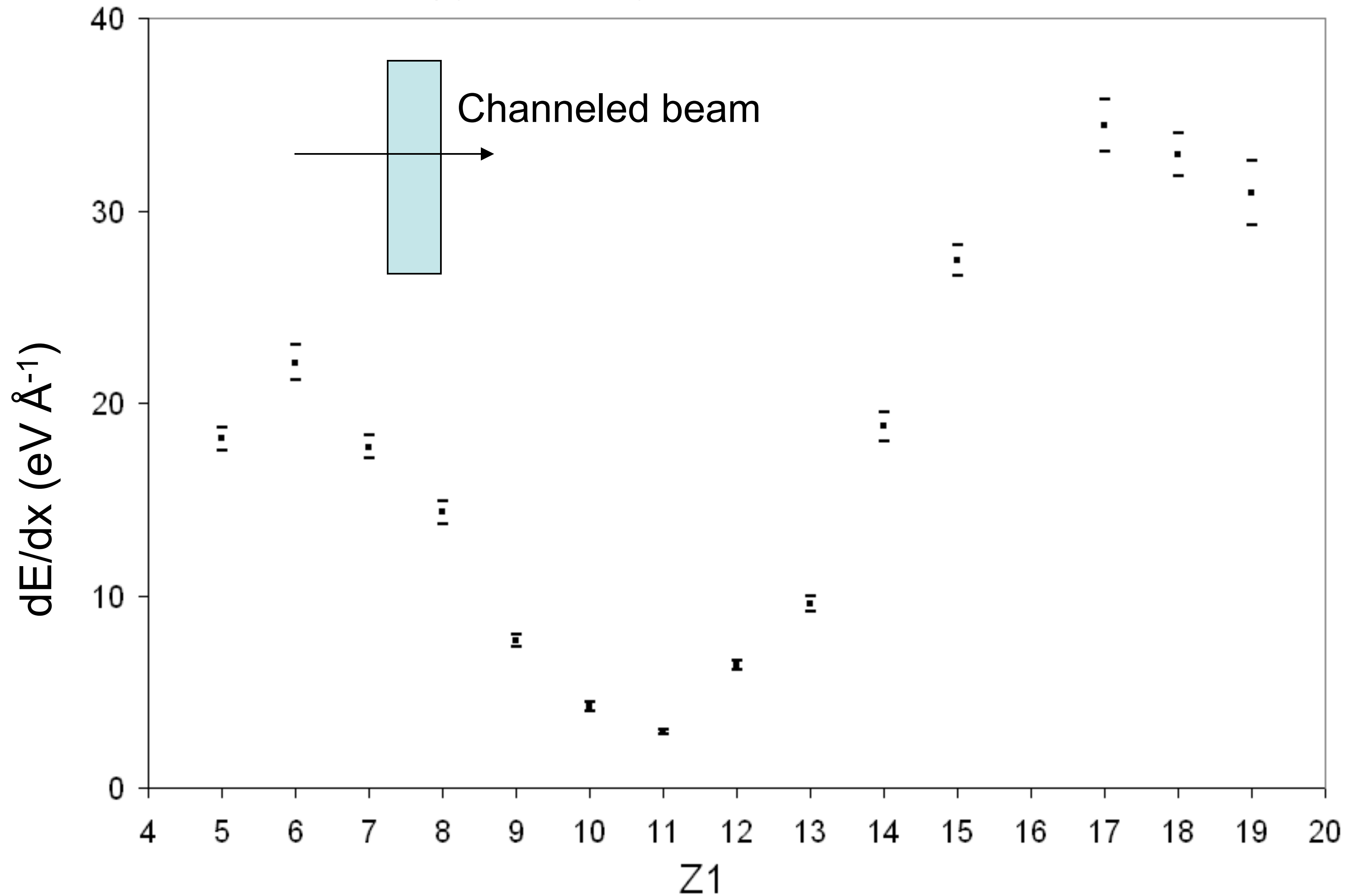
AFOSR/MURI FINAL REVIEW 2010

THEORY OBJECTIVES

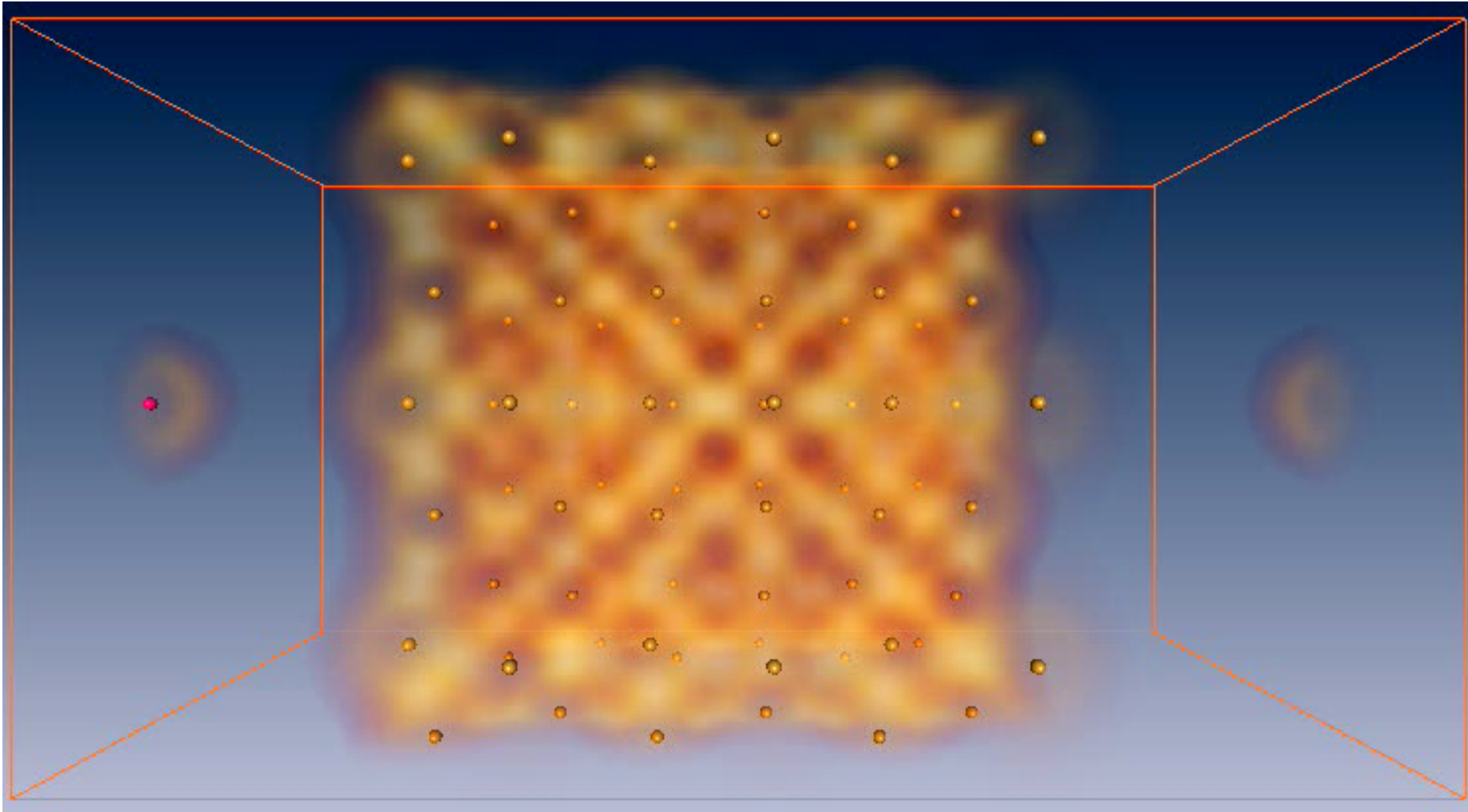
- DISPLACEMENT DAMAGE
  - Defects, charging
  - electrons
- ALTERNATE DIELECTRICS
  - Interface structure, interface defects, NBTI,…
- CARRIER MOBILITIES
- LEAKAGE CURRENTS

Energy loss by channeled ions in Si

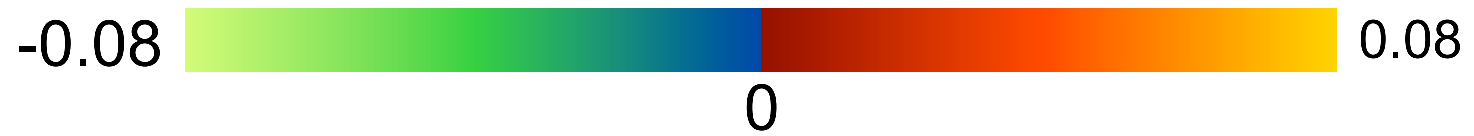


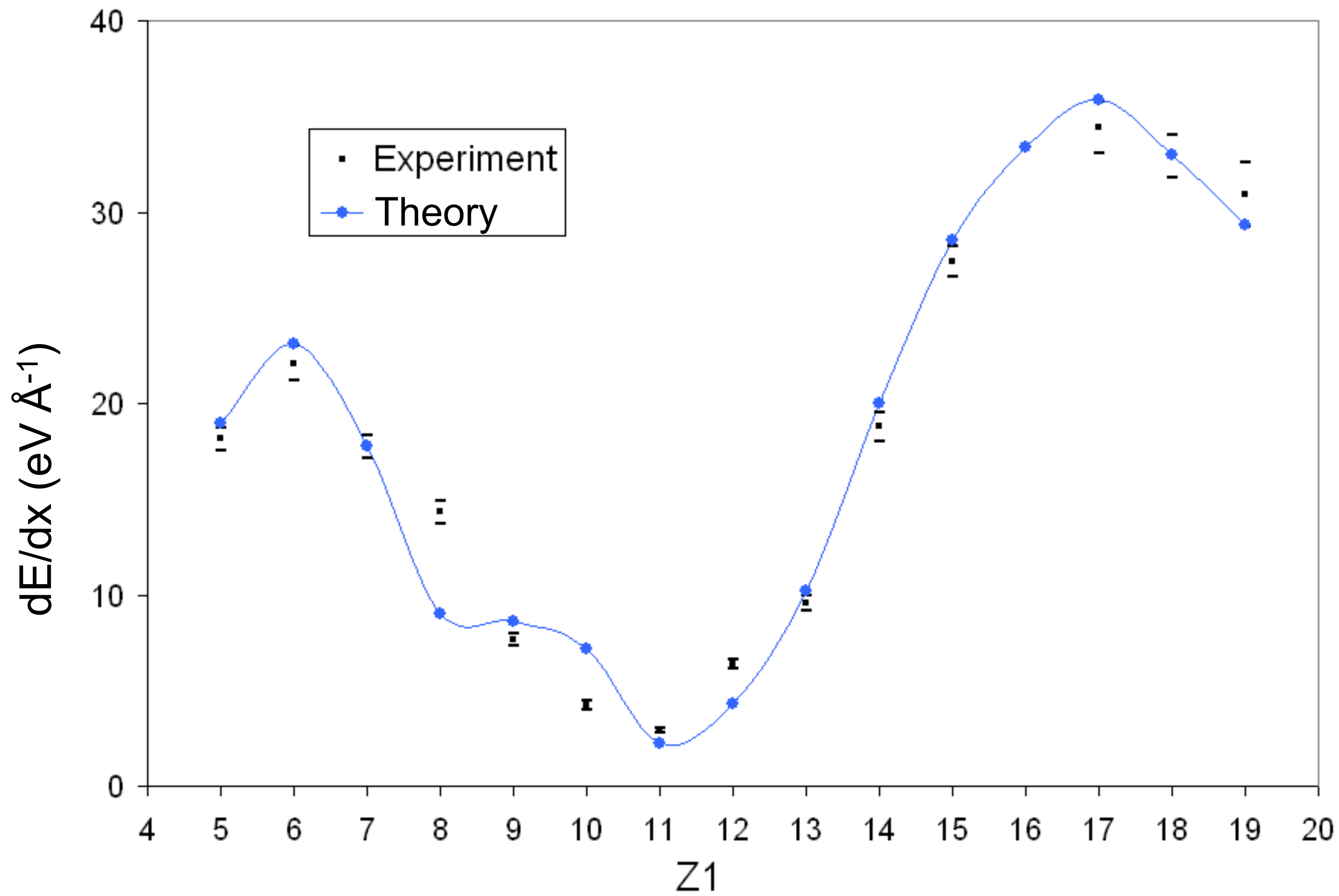
Experimental data, Eisen, 1968

Motion of an ion thru Si<110>



n(t) – n(0)

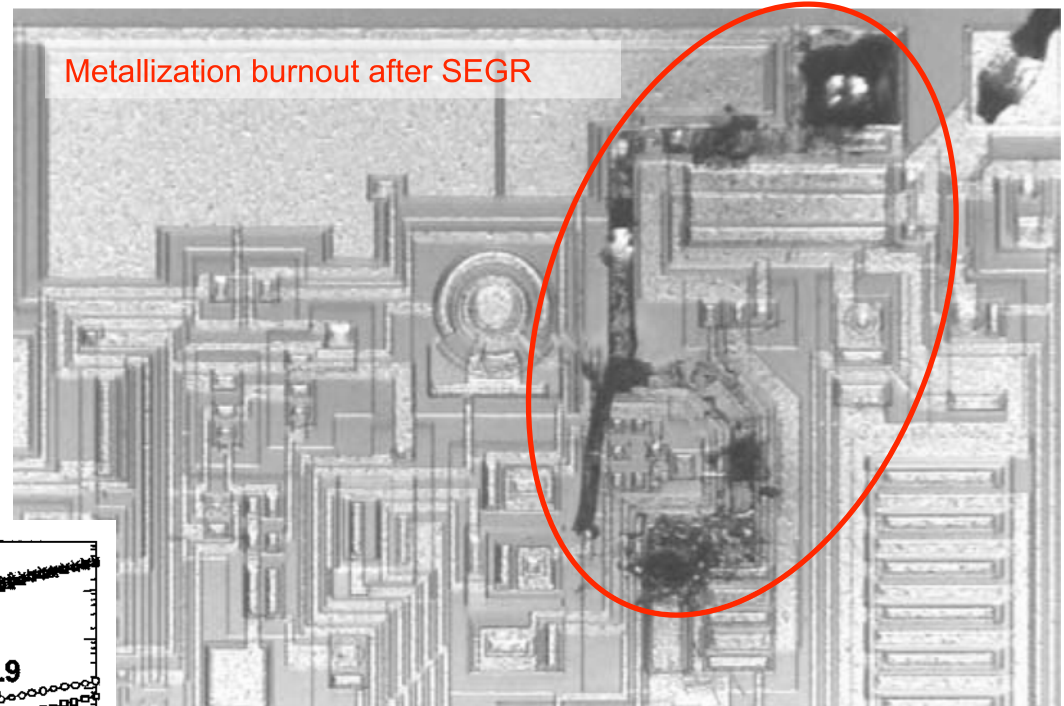




Data: Eisen (1968)

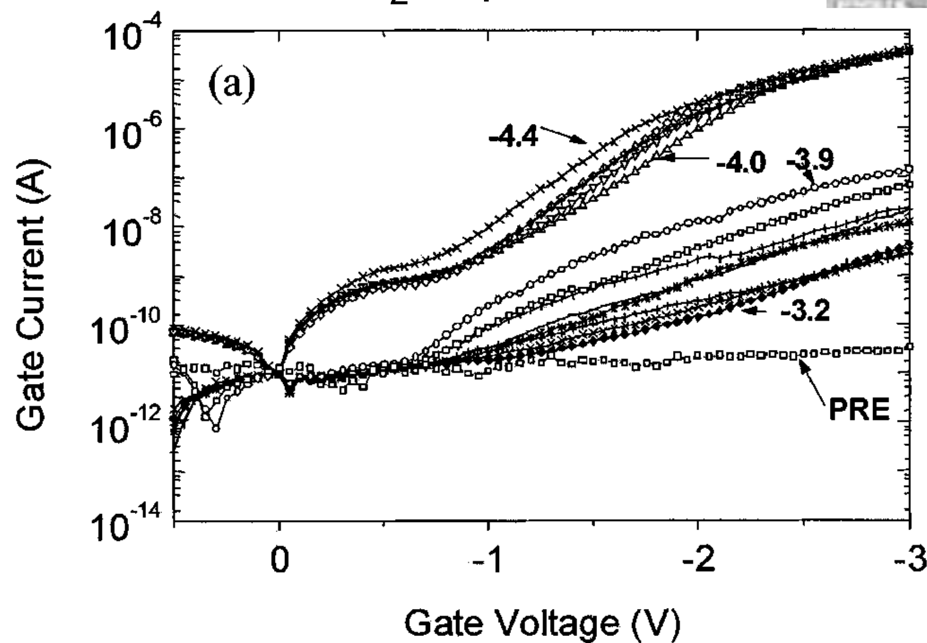
Ryan Hatcher

Single-Event Gate Rupture



Lum et al., IEEE TNS (2004)

I-V following biased irradiation of 3.3 nm SiO_2 capacitors



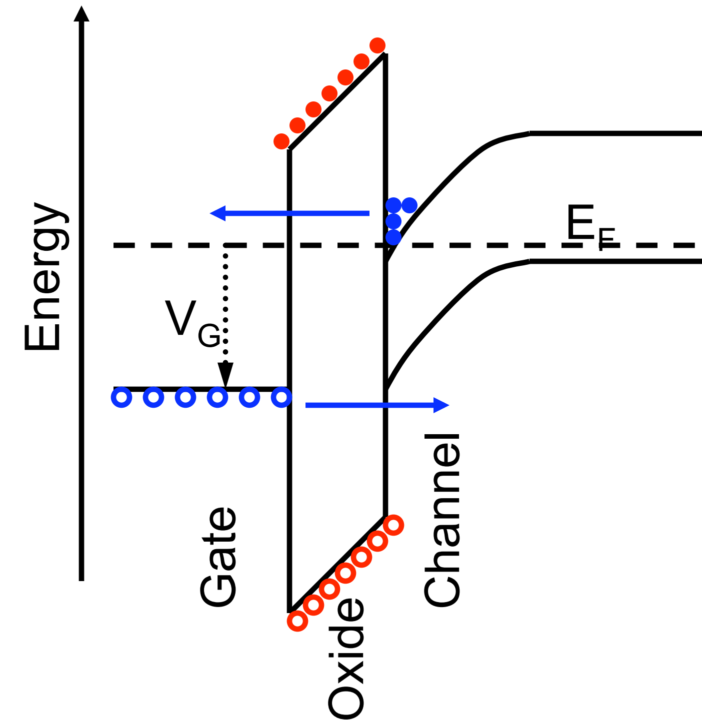
Massengill et al., IEEE TNS (2001)

Leakage-induced rupture

Breakdown results from local heating due to ion-excited carriers…

…AND carriers injected by applied fields

$$\frac{1}{E_{CR}} = \frac{q\mu_1 n(V)}{J_{CR}} + \frac{q\mu_2 n(L)}{J_{CR}}$$

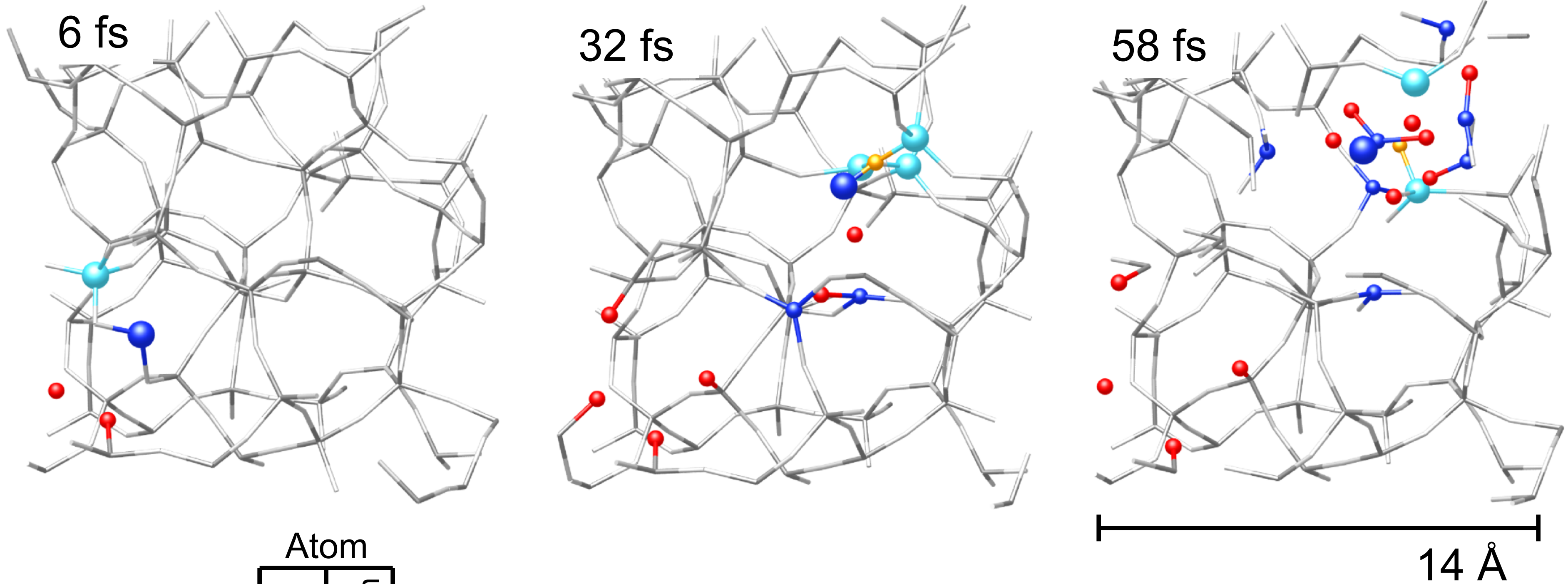


Is it defect mediated?

Sexton, et al., IEEE TNS (1998)

Low-energy recoil dynamics in SiO_2

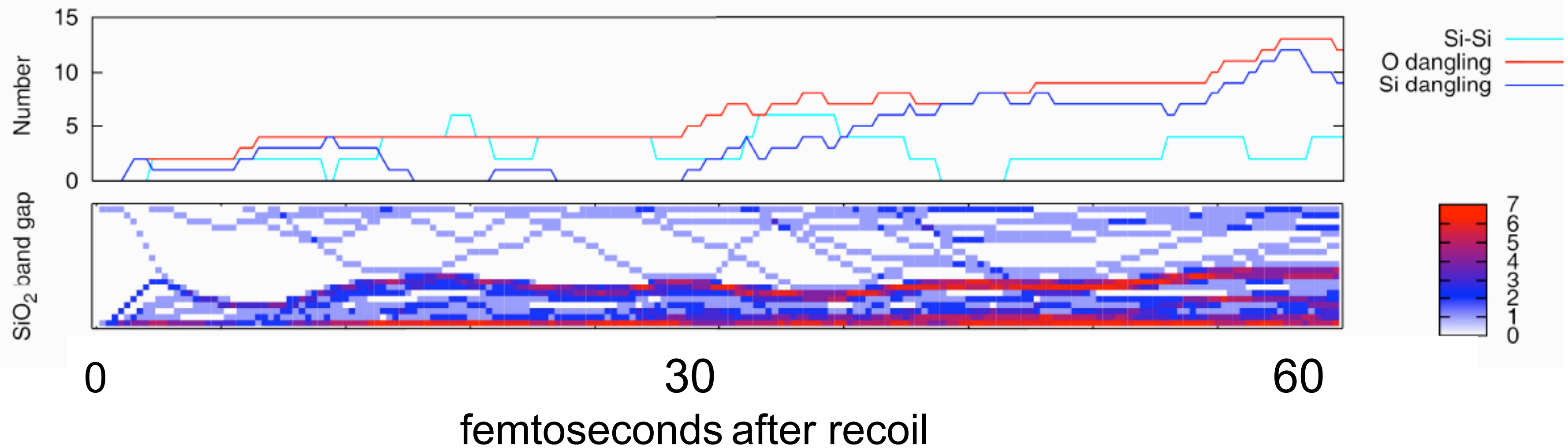
100 eV Si recoil



	Atom	
Defect	Silicon	Oxygen
Dangling Bond	●	●
Extra Bond	●	●
“Self Bond”	Big Ball	

Damage in amorphous material:
Network defects

Defect states in SiO_2

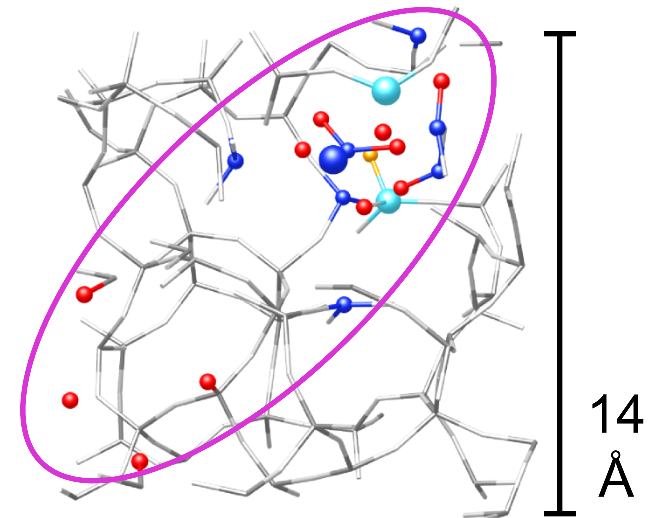


Increasing numbers of defects…

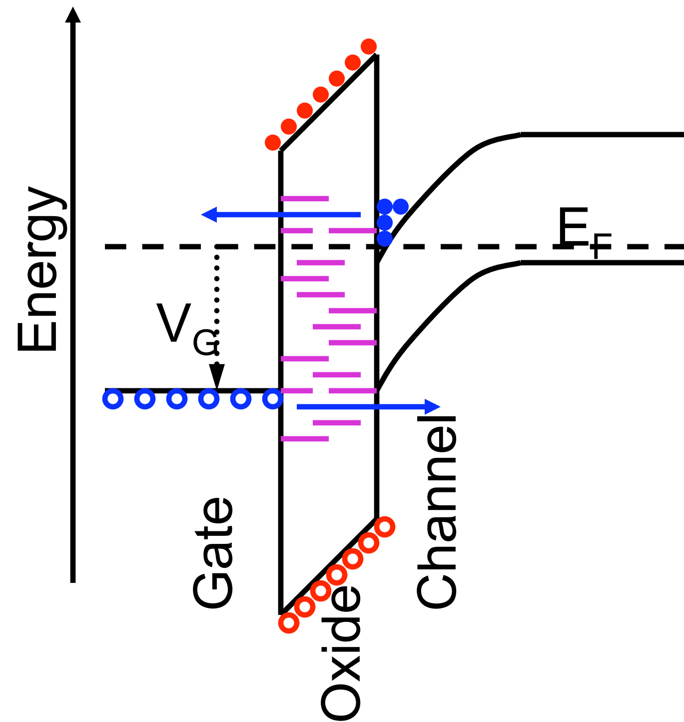
…increasing number of defect states within the bandgap!

Defect states separated by ~2-5 Å!

Conducting path!

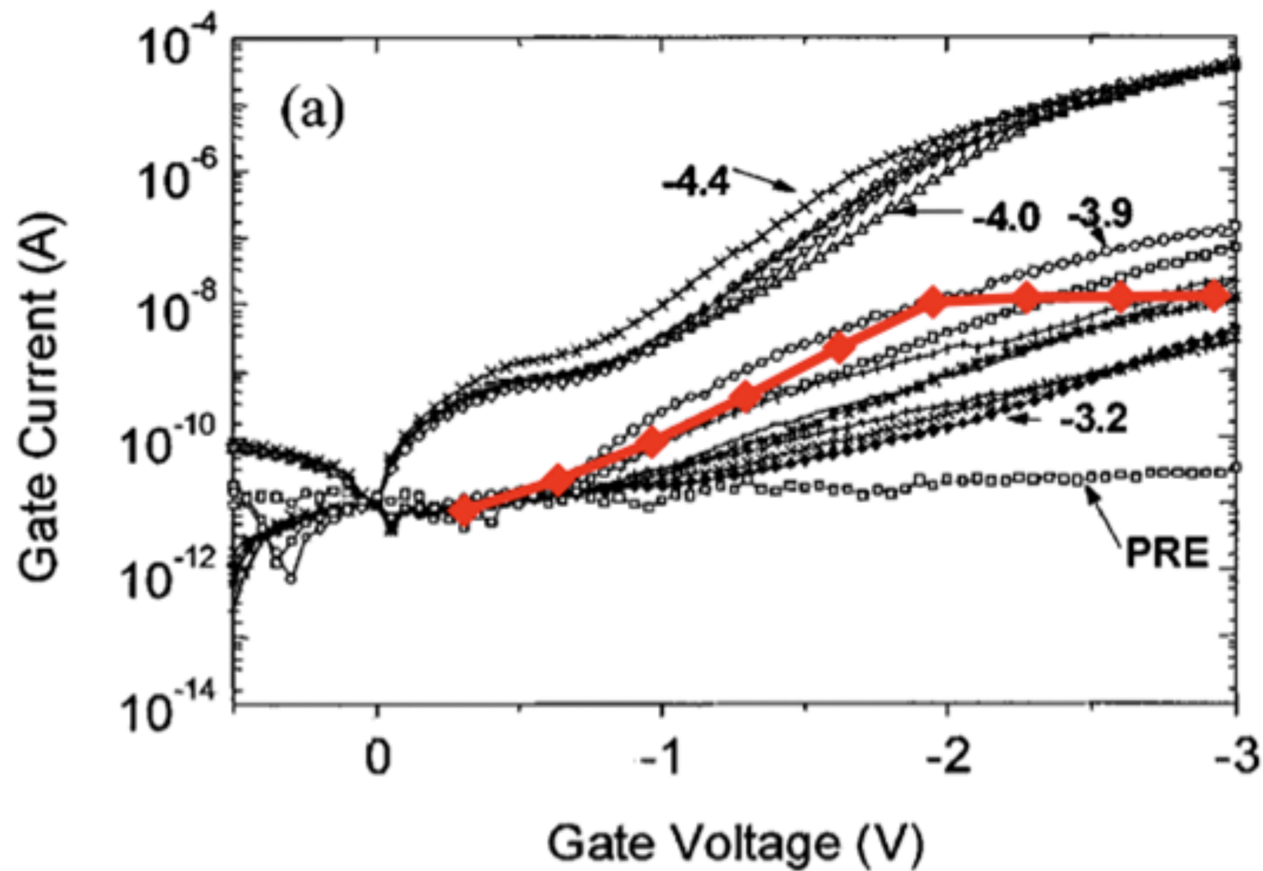


Defect-mediated leakage



Displacement-damage-induced defect states facilitate field-injected leakage

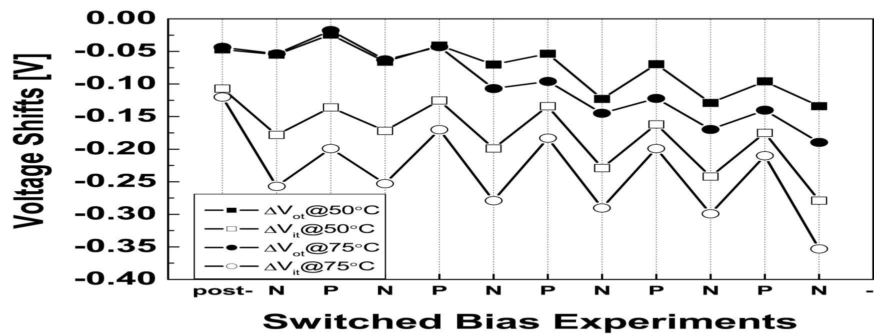
MULTISCALE TRANSPORT THEORY

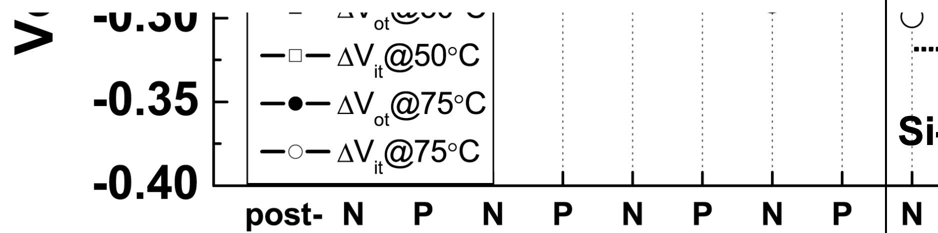


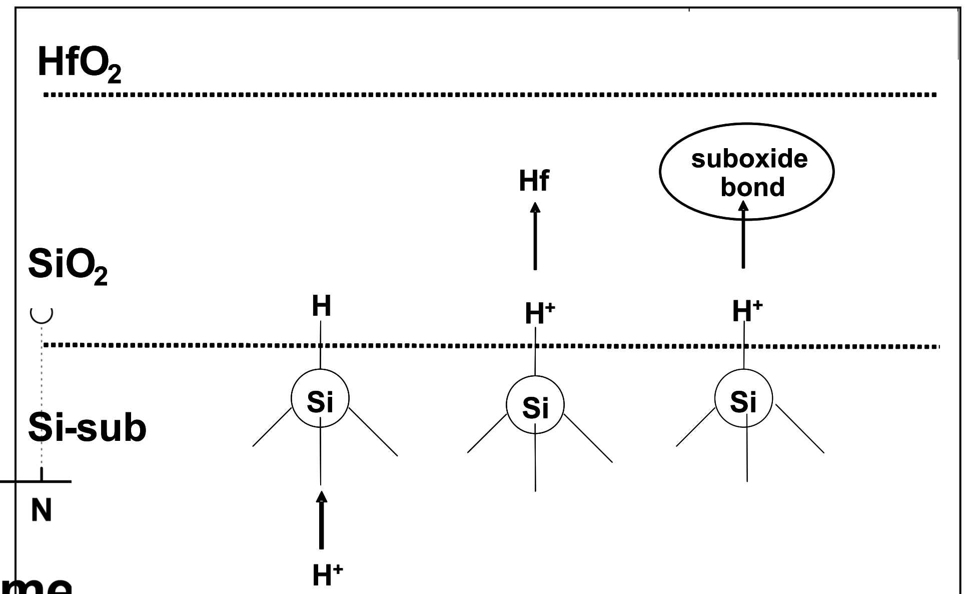
Data by Massengill et al. 2001

Si-SON-HfO_2

POST-IRRADIATION SWITCH-BIAS ANNEALING

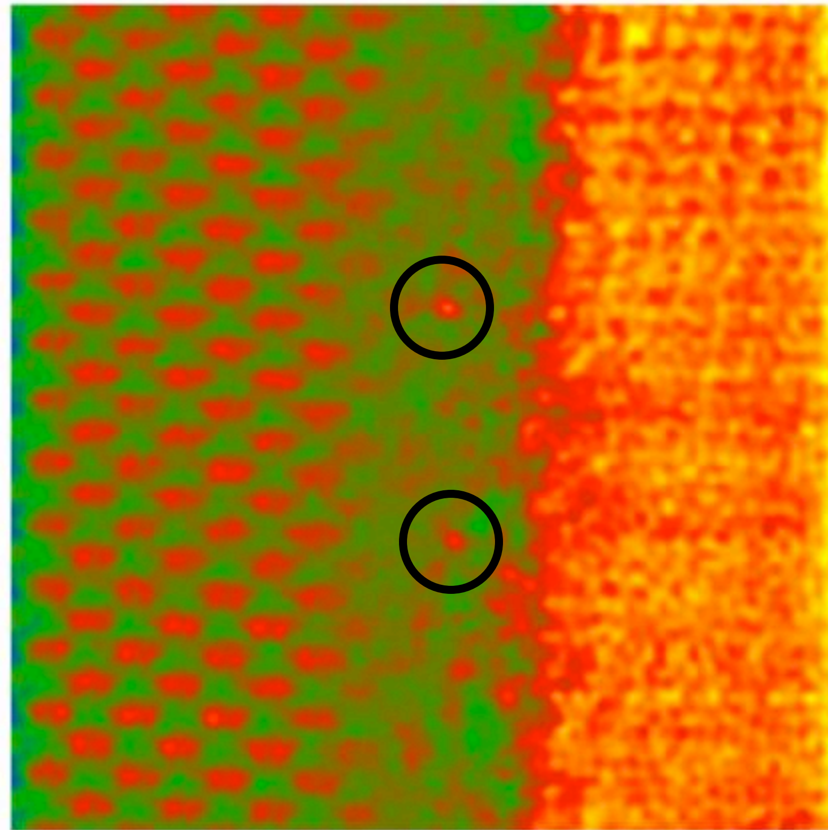






Vanderbilt team

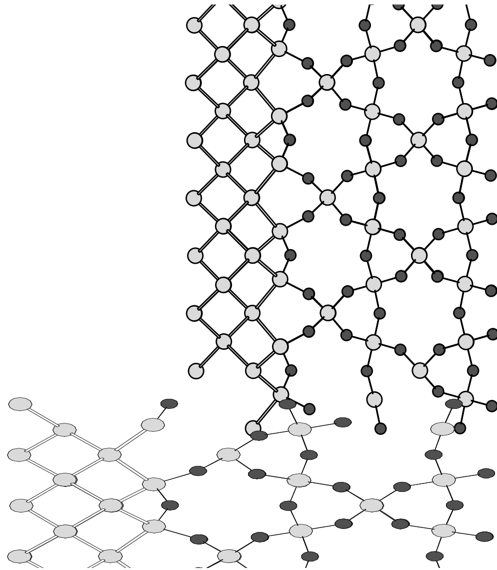
Si SiO_2 HfO_2



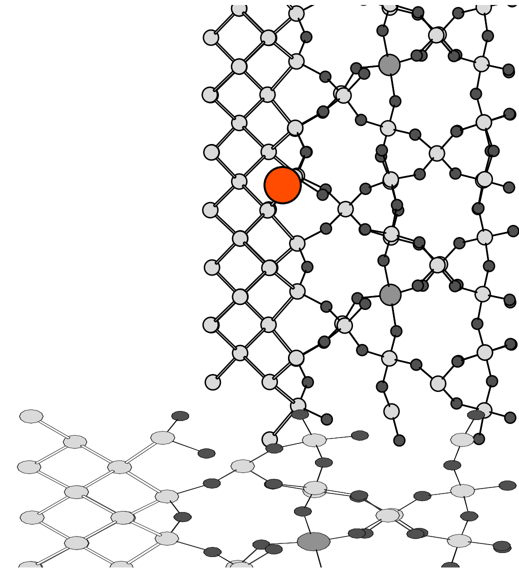
8 Å

Van Benthem & Pennycook, ORNL

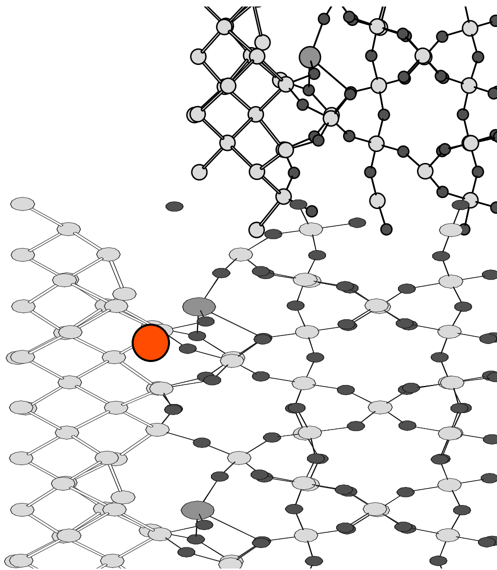
perfect structure



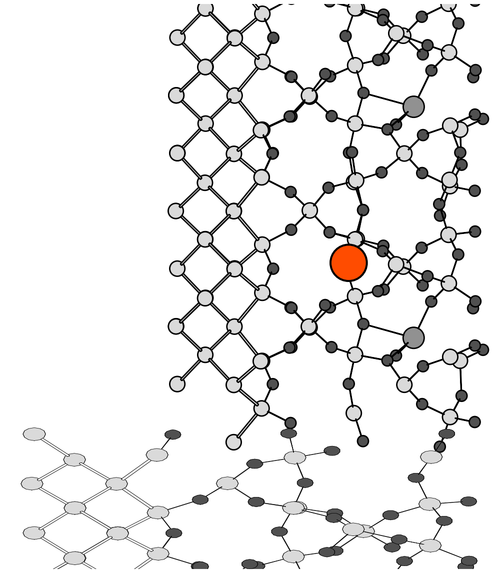
substitutional Hf: local lattice expansion



E(int) = E(sub)+5 eV



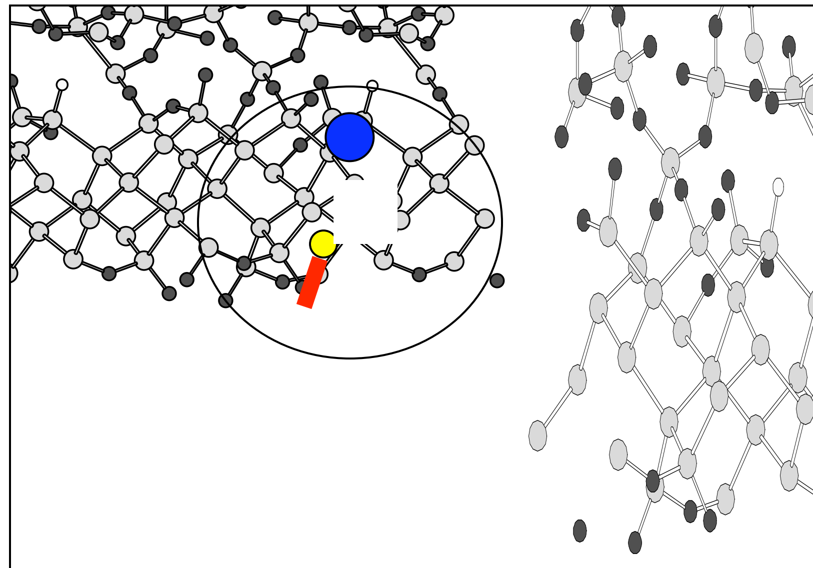
interstitial Hf:
rebonding



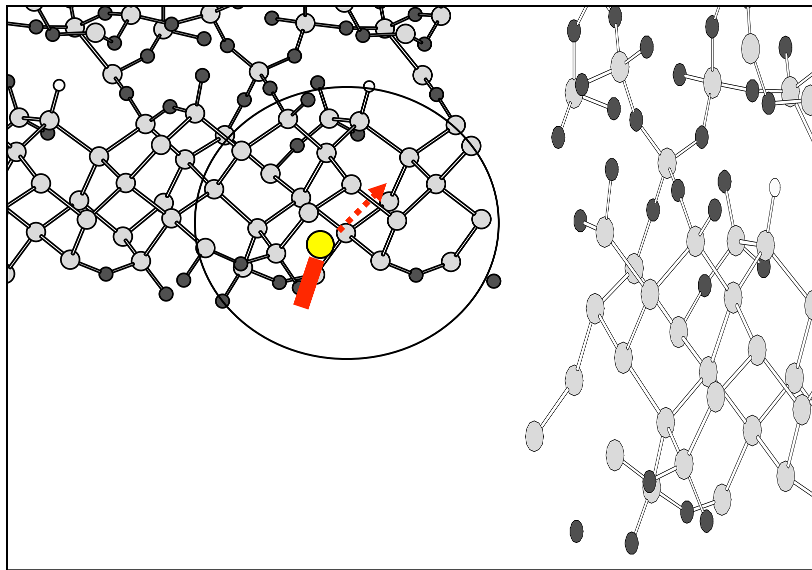
Possible new defect complex

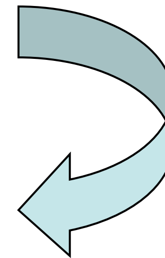
PASSIVATED DB (**Si-H**) ACROSS FROM A SUBOXIDE BOND (Si-Si)

OR Hf-Si BOND

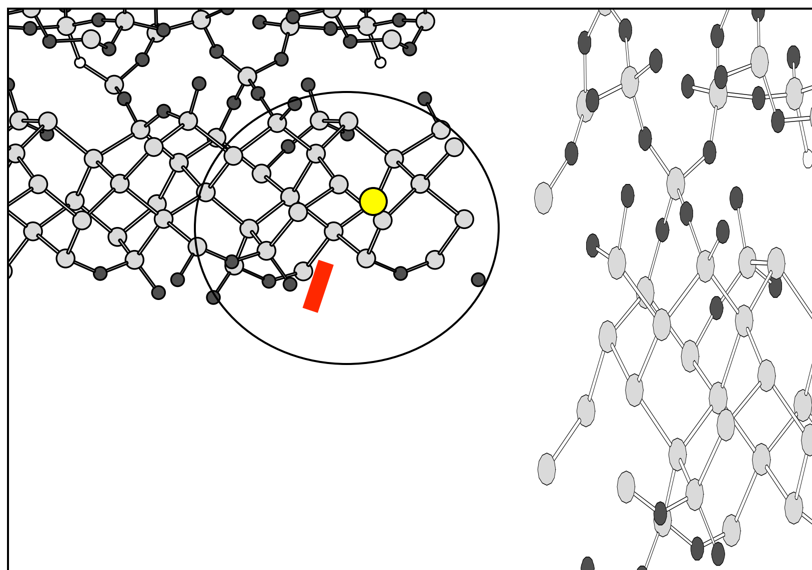


Proton hopping from dangling bond to suboxide bond

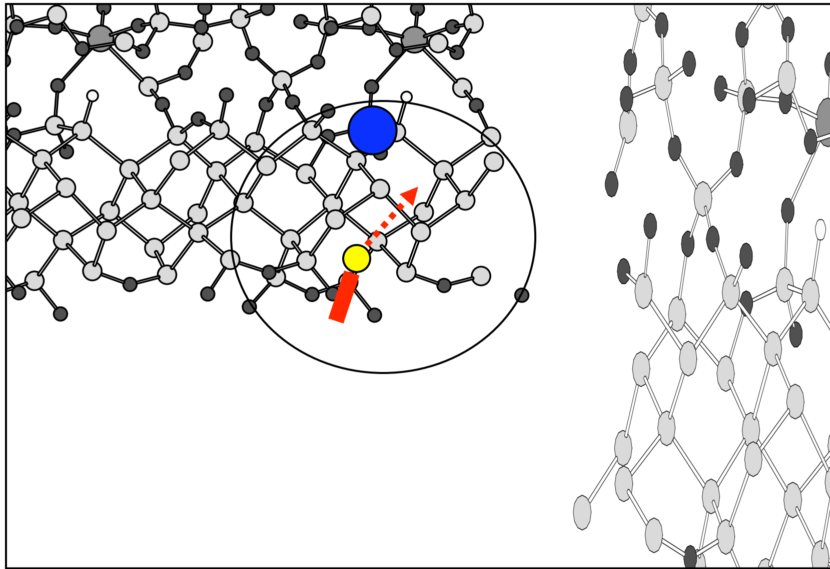


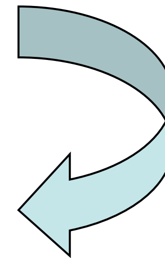


BARRIER > 2.2 eV

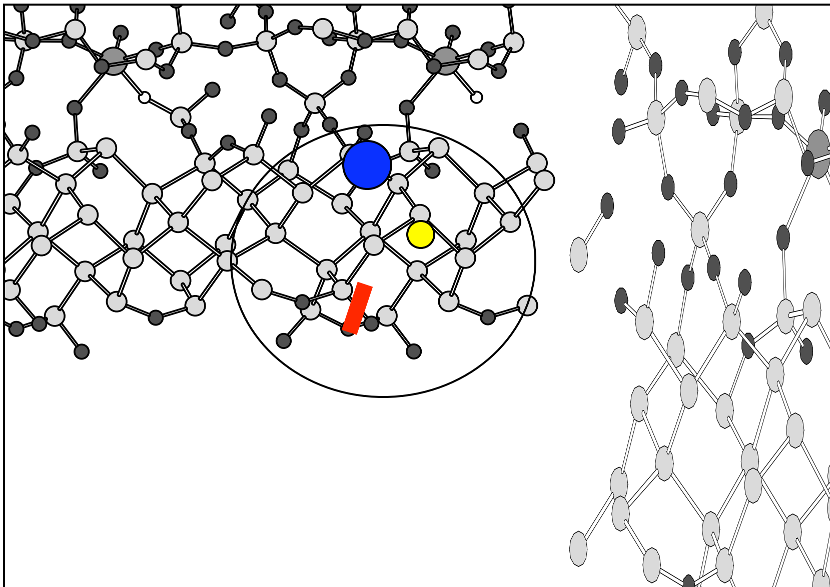


Alternative: DB ACROSS FROM Hf-Si BOND





BARRIER ~ 1.1 eV



NEW RESULTS

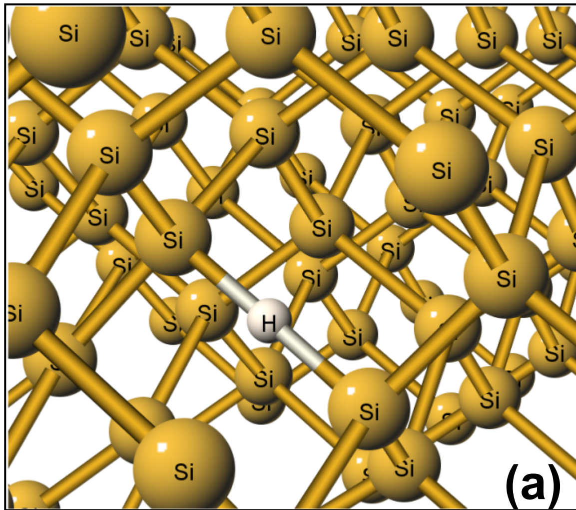
DEFECT DYNAMICS IN SiGe/strained-Si

- FREE HYDROGEN
- PASSIVATION OF DOPANTS BY HYDROGEN
- VACANCIES AND INTERSTITIALS

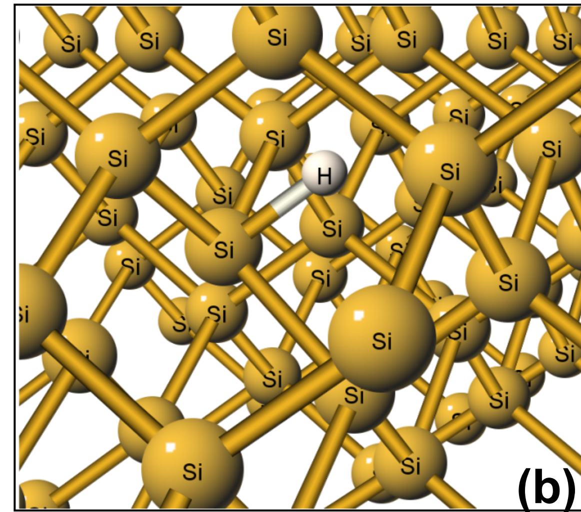
L. Tsetseris, D. M. Fleetwood, R. D. Schrimpf, and S. T. Pantelides,
submitted to Appl. Phys. Lett.

Hydrogen in SiGe and strained Si

H^0, H^+



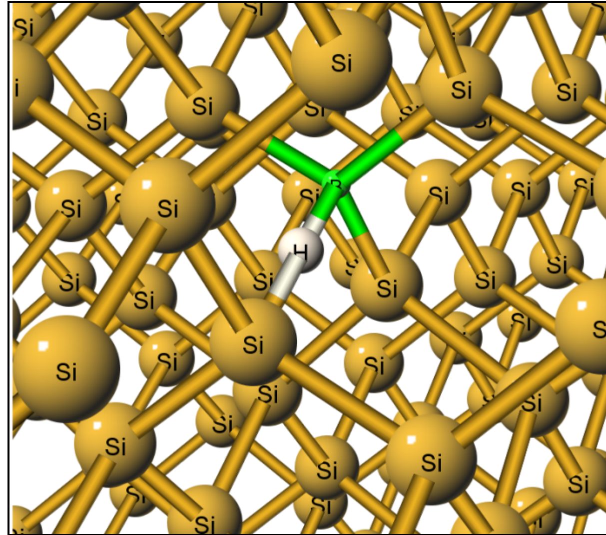
H^-



x_{Ge}	Charge	ΔE (eV)
11.1%	0	0.01
22.2%	0	0.07
33.3%	0	0.05

H^0 prefers SiGe

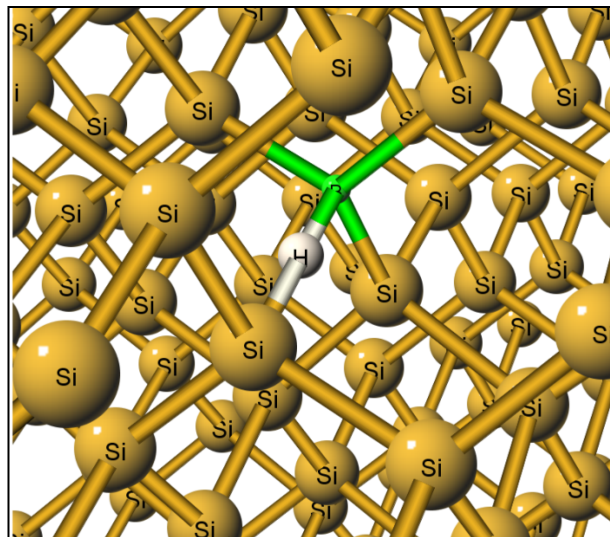
Hydrogen-boron complexes in SiGe and s-Si



x_{Ge}	Charge	E_b (eV)	ΔE (eV)
11.1%	0	0.61	0.00
22.2%	0	0.63	-0.22
33.3%	0	0.57	-0.54

H prefers to stick to B in s-Si.

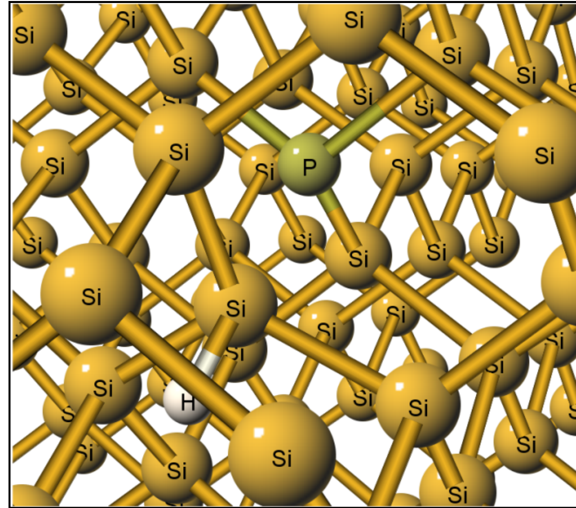
Hydrogen-boron complexes in SiGe and s-Si



x_{Ge}	Charge	E_b (eV)	ΔE (eV)
11.1%	0	0.61	0.00
22.2%	0	0.63	-0.22
33.3%	0	0.57	-0.54
11.1%	-	0.48	0.00
22.2%	-	0.54	-0.08
33.3%	-	0.44	-0.13

H prefers to stick to B in s-Si.

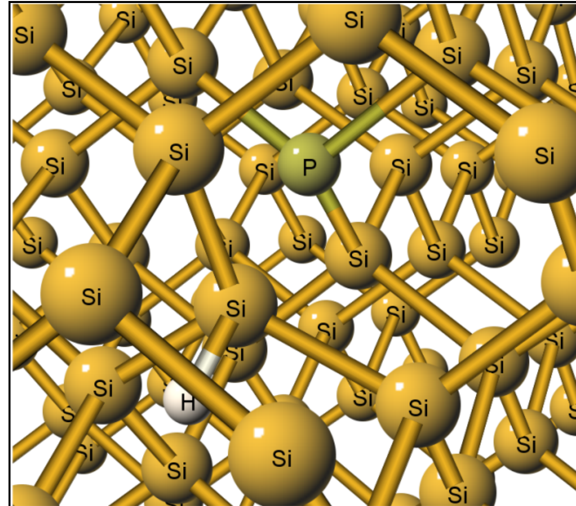
P-H complexes in SiGe and s-Si



x_{Ge}	Charge	E_b (eV)	ΔE (eV)
11.1%	0	0.70	0.00
22.2%	0	0.45	0.18
33.3%	0	0.52	0.42

H prefers to stick to P sites in SiGe.

P-H complexes in SiGe and s-Si



x_{Ge}	Charge	E_b (eV)	ΔE (eV)
11.1%	0	0.70	0.00
22.2%	0	0.45	0.18
33.3%	0	0.52	0.42
11.1%	+	0.31	0.00
22.2%	+	0.27	0.01
33.3%	+	0.30	0.01

H prefers to stick to P sites in SiGe.

IMPACT ON DEVICE OPERATION

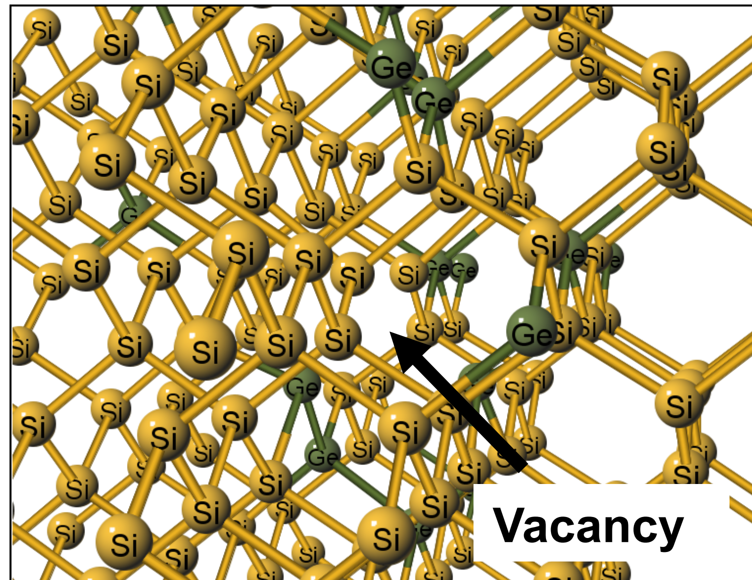
NBTI, PBTI

INCREASE IN INTERFACE TRAP DENSITY
BIAS, MODERATE TEMPERATURES (~150° C)

H prefers to stick to B in s-Si
BTI GETS WORSE

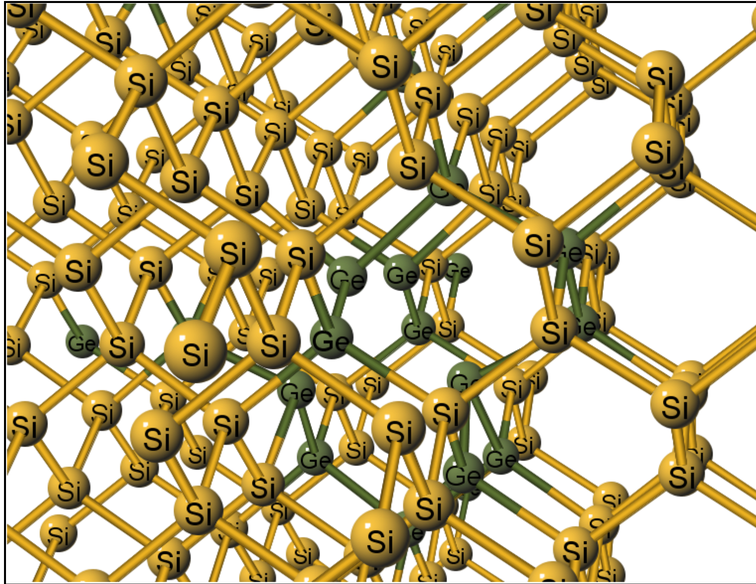
H prefers to stick to P sites in SiGe
BTI IMPROVEMENT

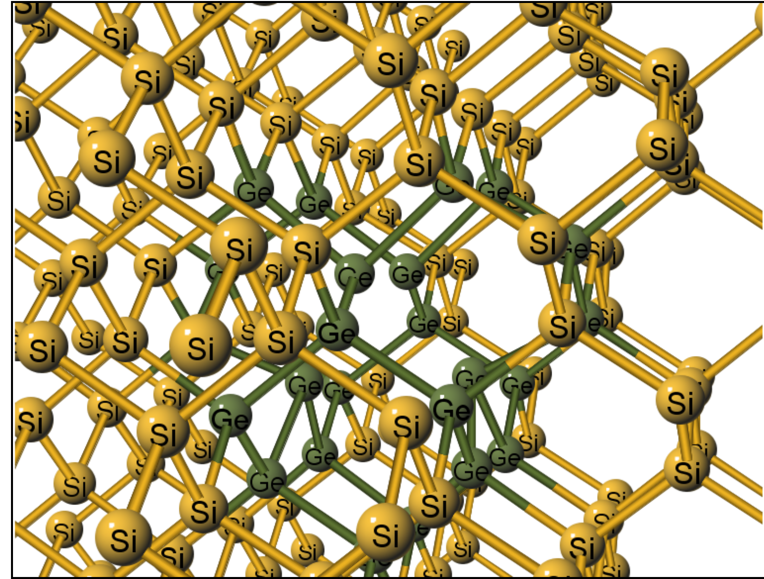
Vacancies in SiGe/strained Si

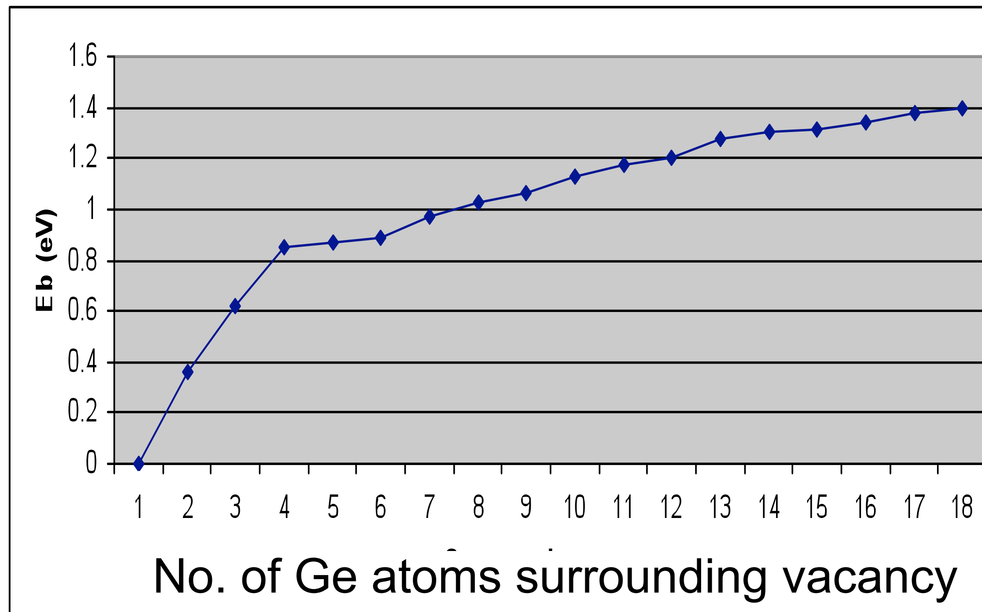


Vacancies have lower energy in SiGe

Agglomeration of Ge atoms around vacancies in SiGe

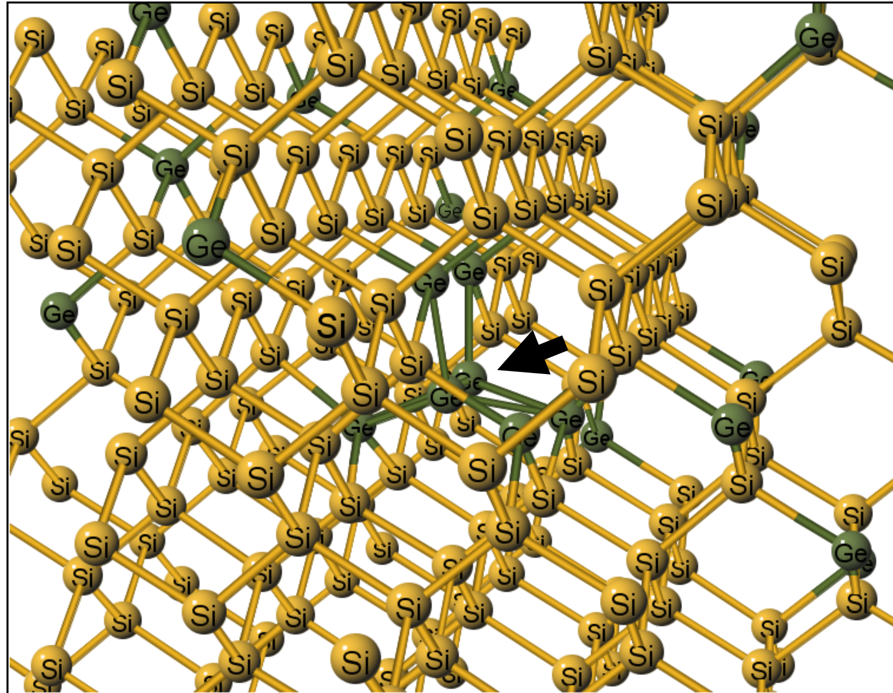






1.4 eV

Self-interstitials in SiGe/strained Si



- Si self-interstitial moves from s-Si to SiGe
  energy gain 0.23 eV for x_{Ge} = 11%

- Si interstitial goes substitutional, creating a Ge interstitial

- Ge atoms agglomerate around Ge self-interstitial
  (trend weaker than that for vacancies)

IMPACT ON DEVICE OPERATION

PRESENCE OF SiGe SUBSTRATE REDUCES

RADIATION-INDUCED DISPLACEMENT DAMAGE

Ge/high-k systems
Ge volatilization products in high-k dielectrics

- **Annealing of Ge substrates initiates volatilization and desorption of GeO molecules**

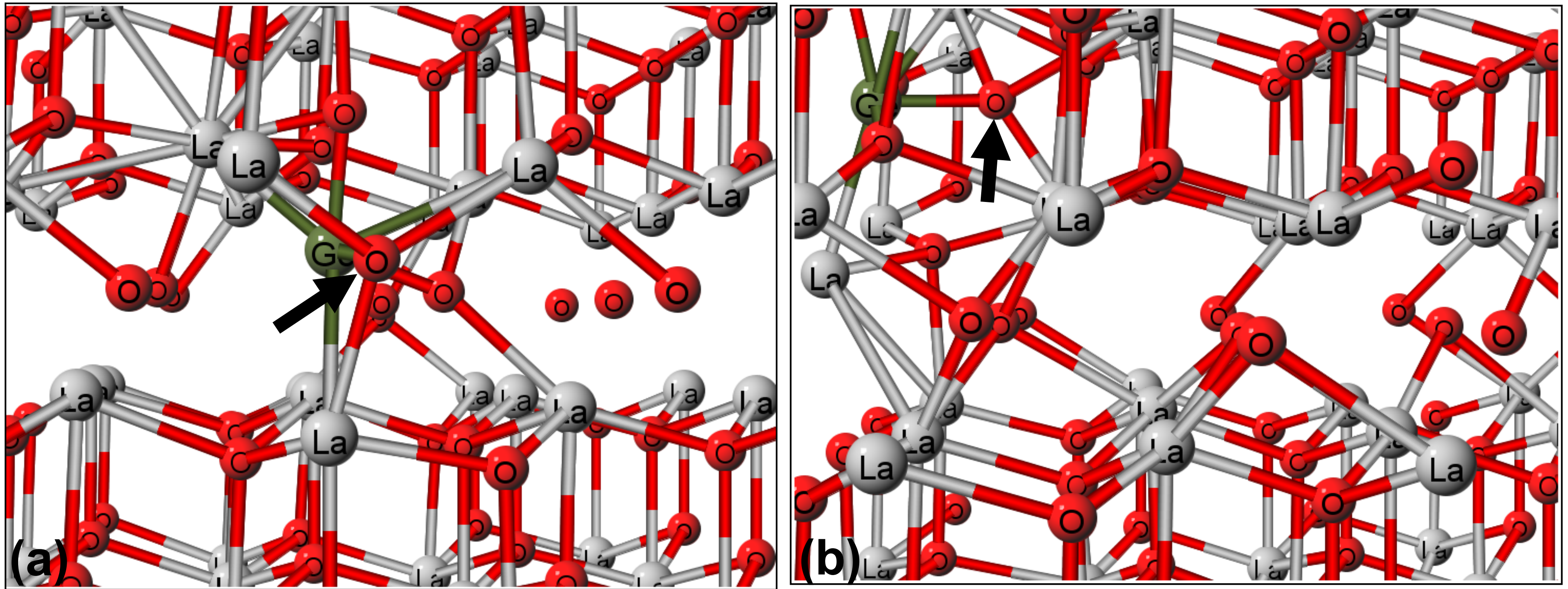
- **In Ge-based gate stacks, GeO must out-diffuse through the gate dielectric**

- **Some of the GeO molecules may be trapped in the gate oxides**

- **Experimental evidence: out-diffusion of Ge-related species causes degradation of the dielectric (e.g. charge trapping, enhanced leakage current)**

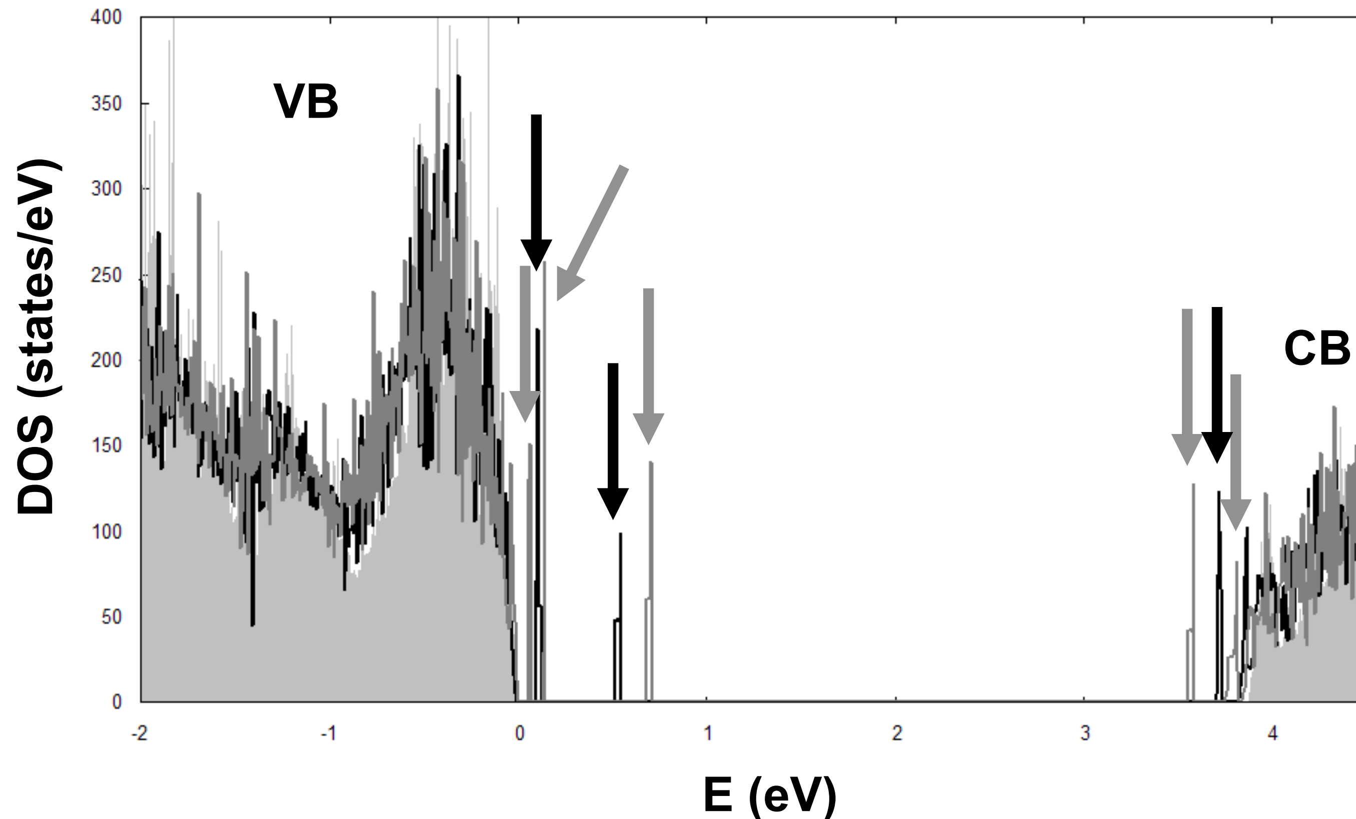
V. Golias, L. Tsetseris, A. Dimoulas, and S. T. Pantelides, Microelectr. Eng., submitted

GeO impurities in La_2O_3



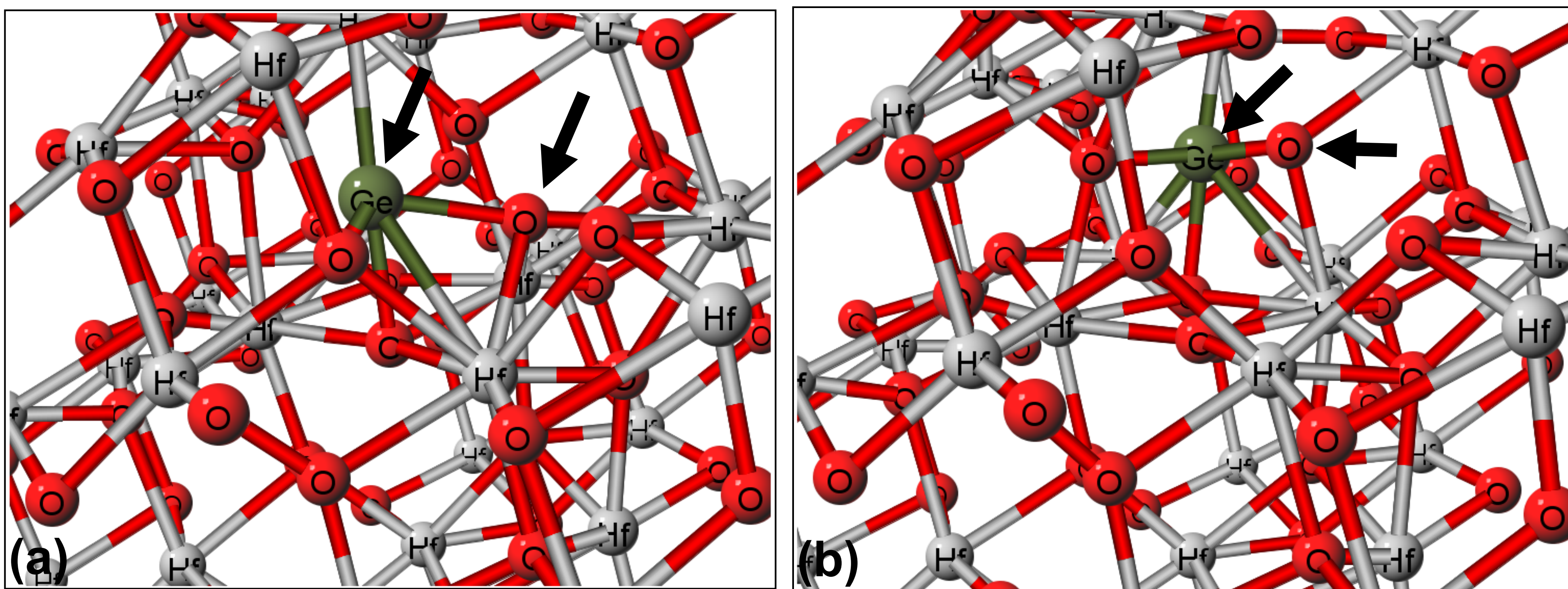
- Hex-La_2O_3: layered structure with La-rich slices and O atoms in-between.
- Stable configurations of GeO impurities within and inside the layers.
- GeO transfer from La_2O_3 bulk to vacuum: energy gain of 2.7 eV

GeO in La_2O_3: Electronic properties



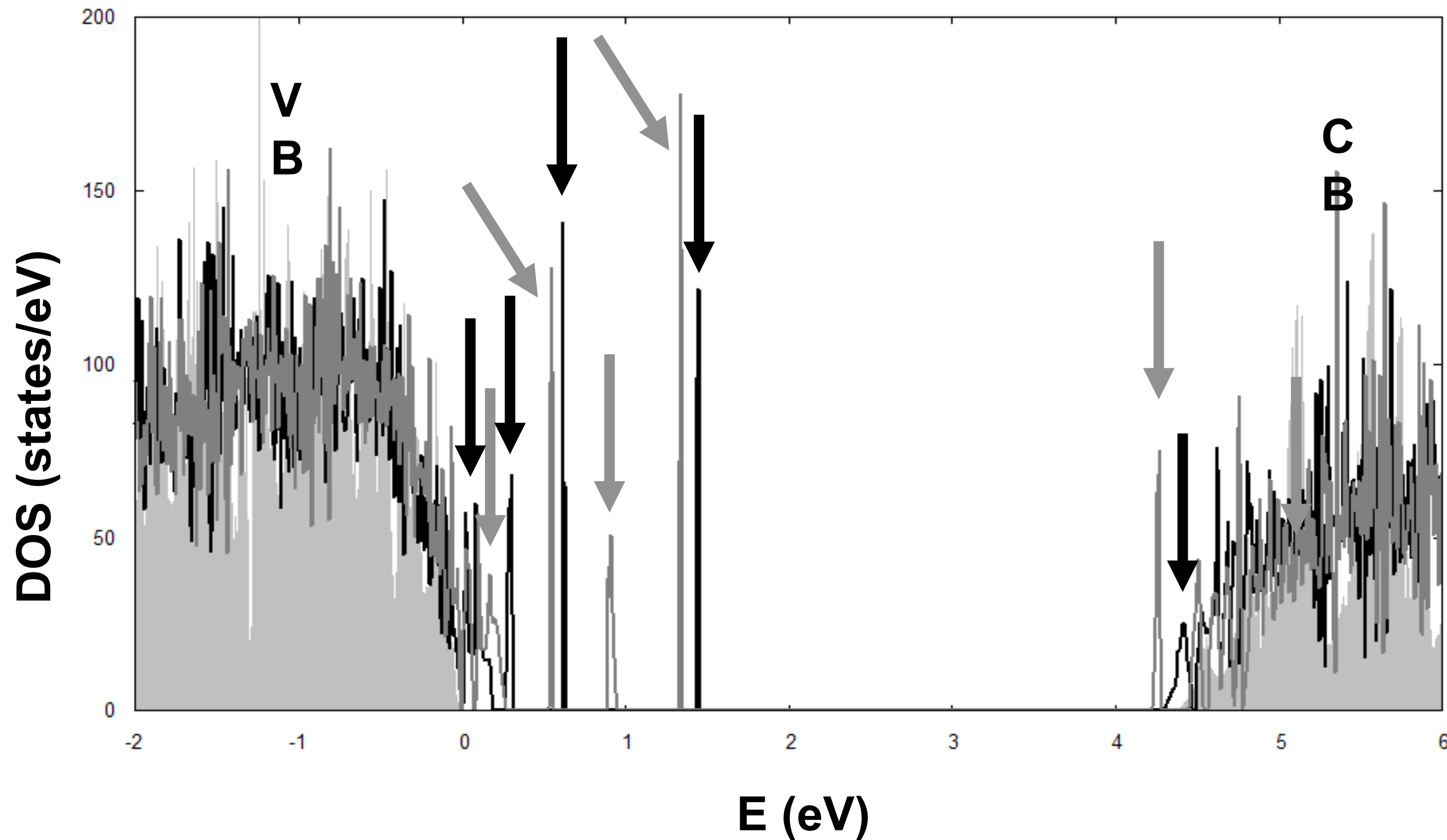
- Energy levels in the gap cause **charge trapping** and enhance **leakage currents**
- Hydrogen binds to GeO impurities, but some levels in the gap remain

GeO impurities in HfO_2



GeO transfer from HfO_2 bulk to vacuum: energy gain of 1.5 eV

GeO in HfO_2: Electronic properties



- Energy levels in the gap cause **charge trapping** and enhance **leakage currents**
- Hydrogen binds to GeO impurities, but some levels in the gap remain

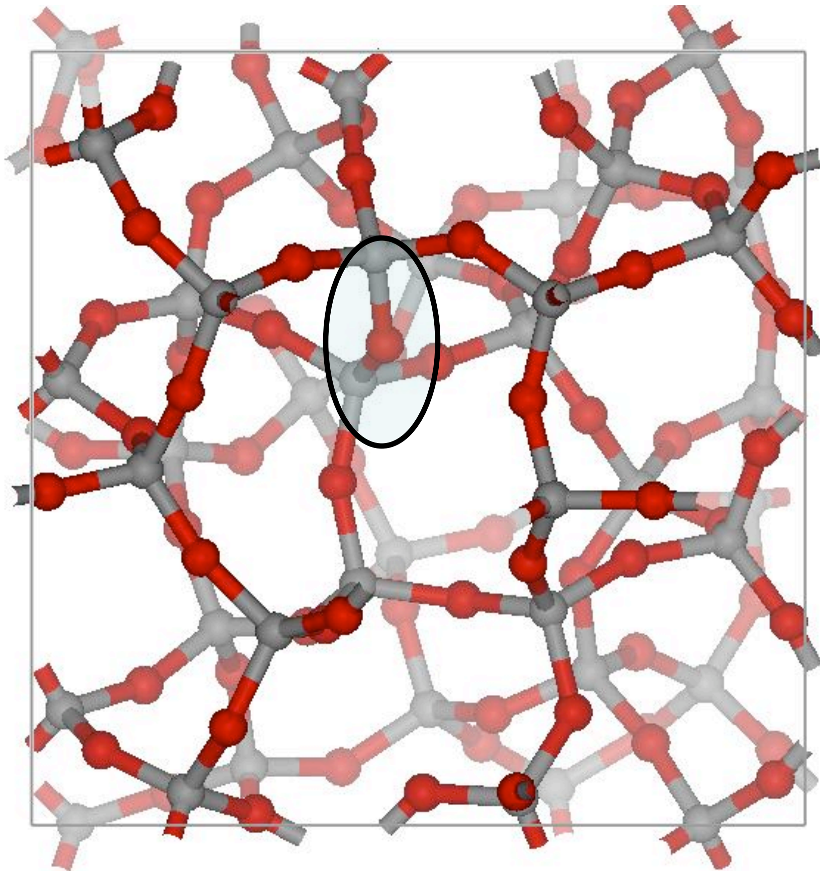
CRACKING OF H_2 IN SiO_2

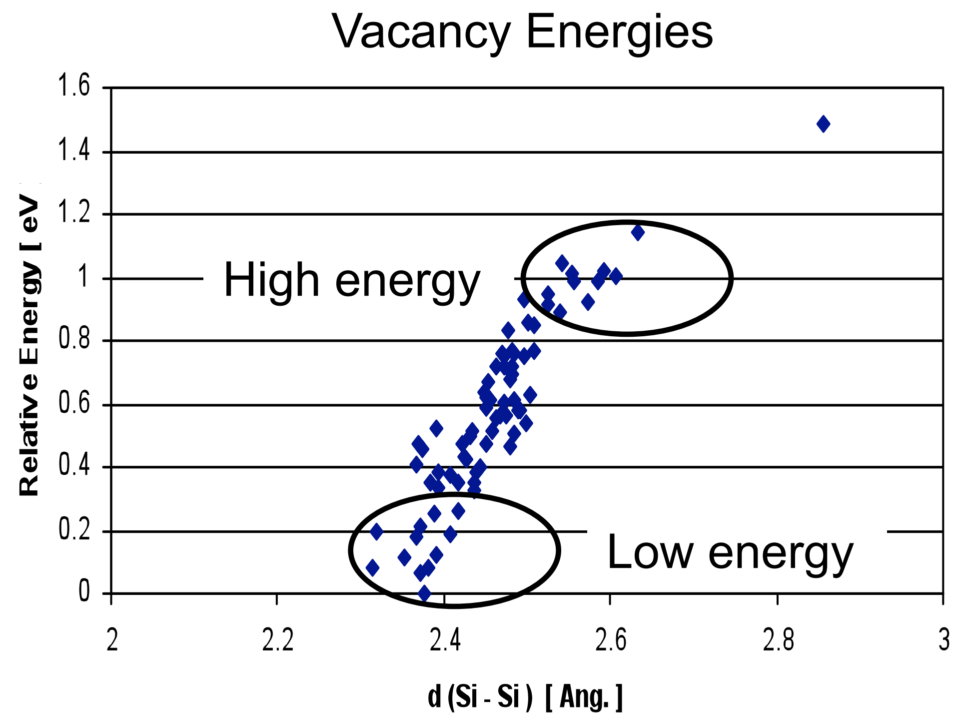
- Conley and Lenahan (1993):

Experimental evidence in support of H_2 cracking at O vacancies

- Contrary to theoretical results
(Edwards and coworkers 1992,1993)

Oxygen Vacancies

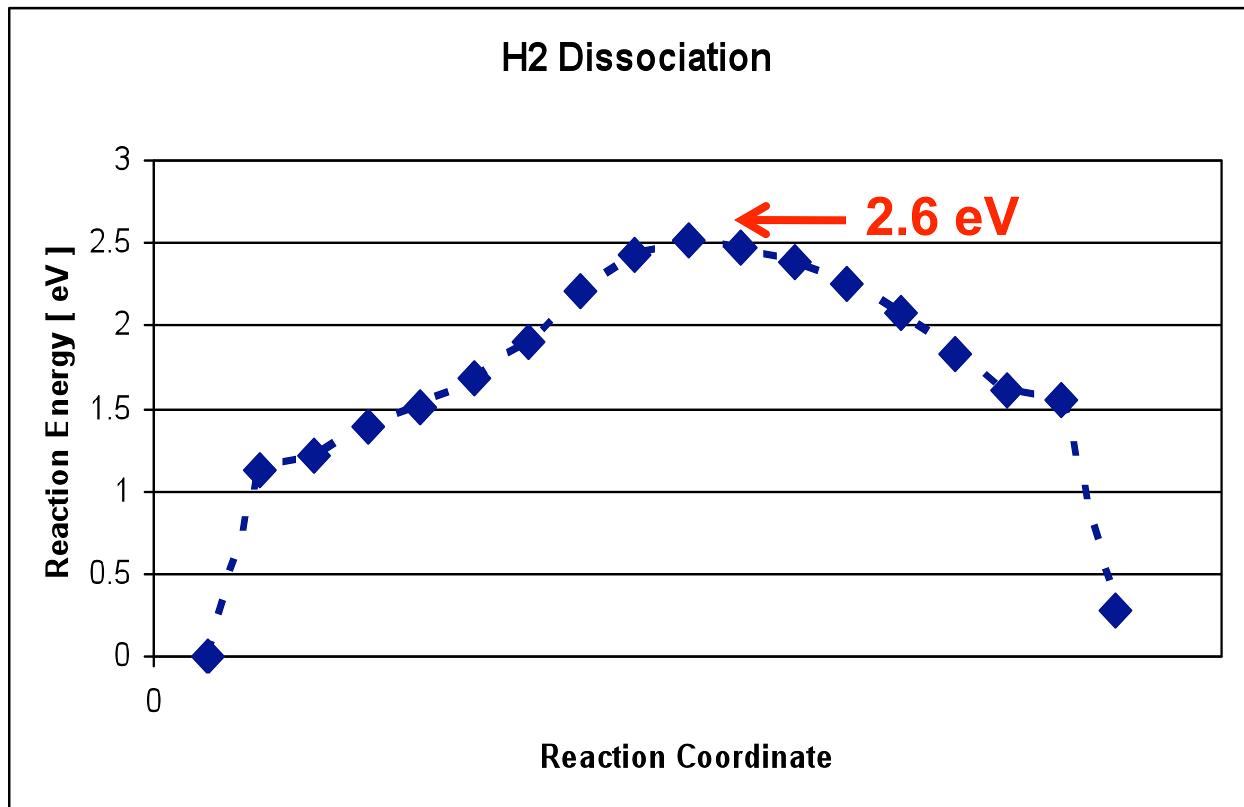




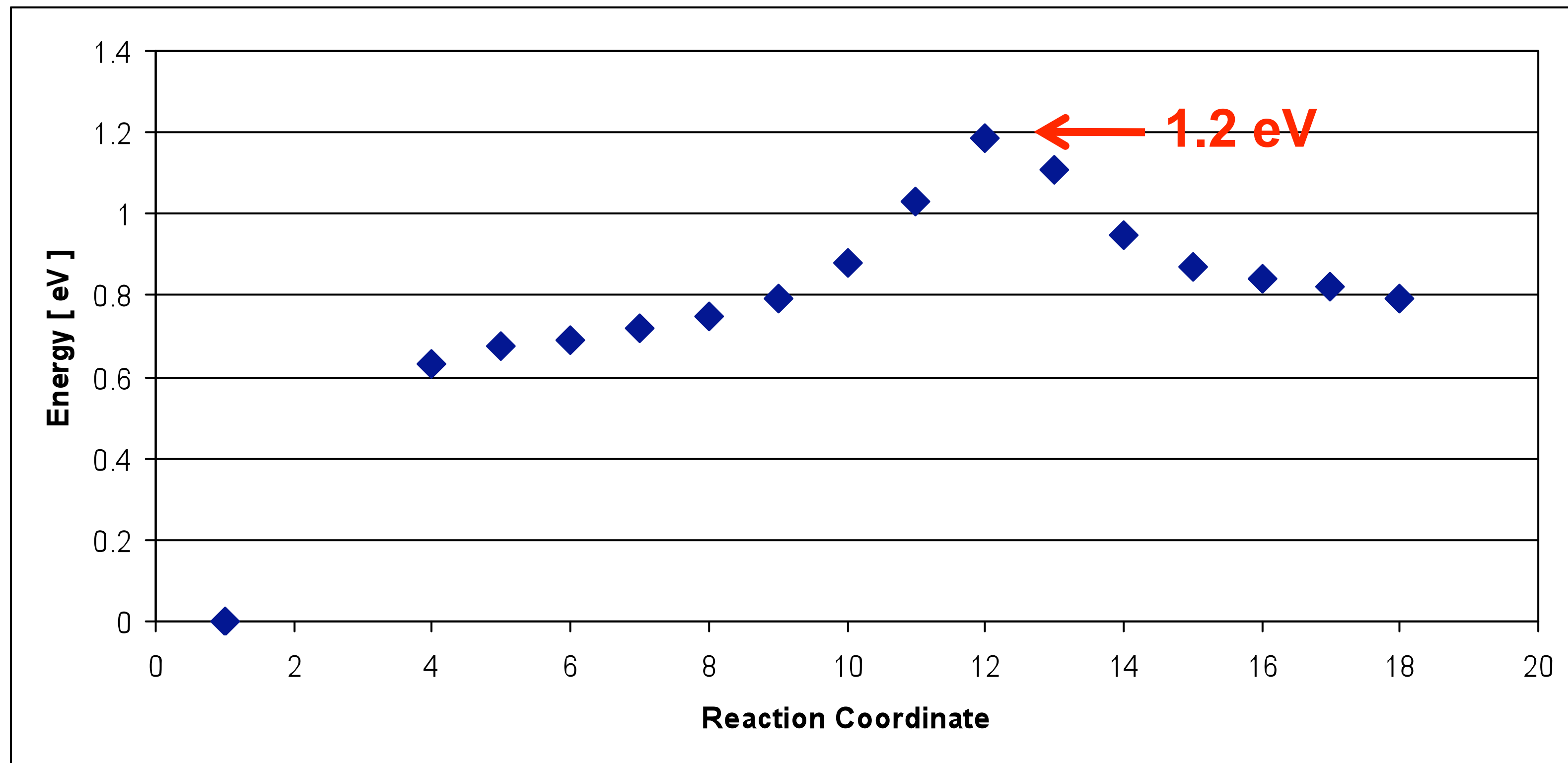
T ~ 1200 K

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

H_2 reacting at V

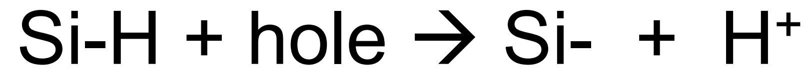


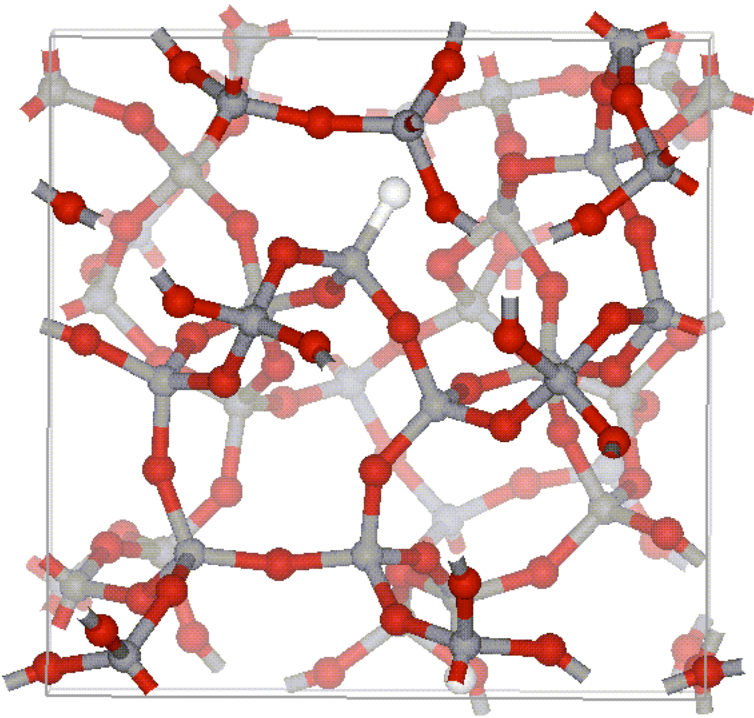
H_2 reacting at V^+

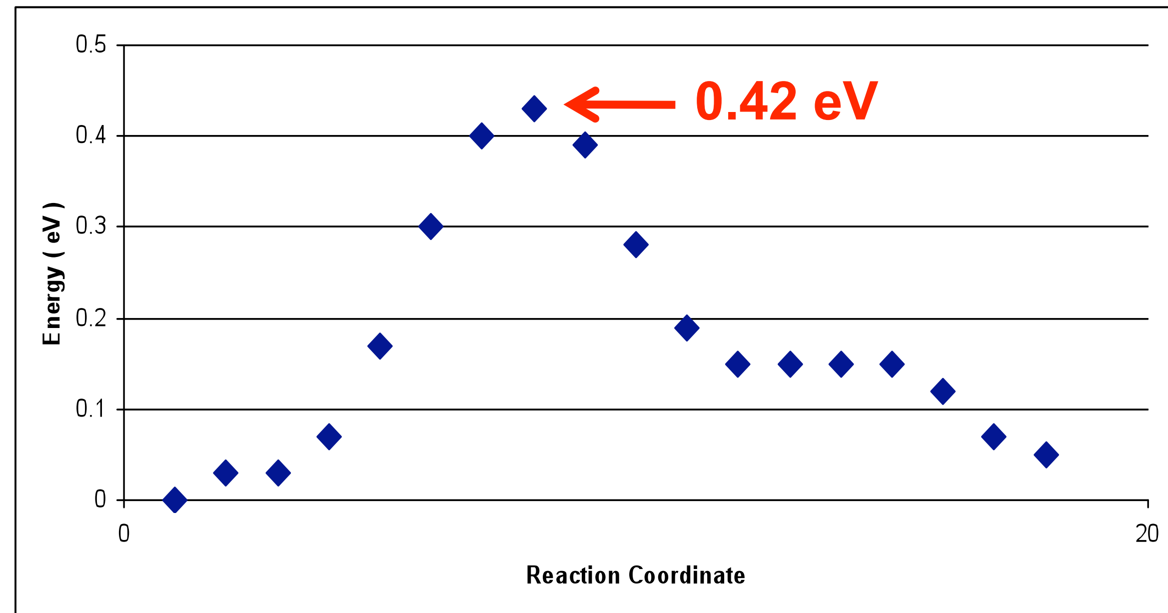


H_2 does not crack at room temperature at low-energy vacancies!

ALTERNATIVE MECHANISM: Si DANGLING BONDS







H_2 cracks at a bare dangling bond
without an energy barrier